

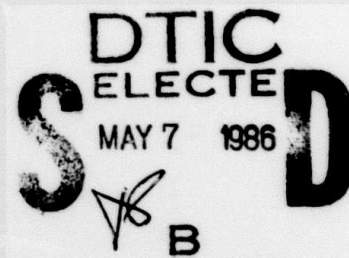
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CONTRACTOR REPORT

GAS DYNAMICS OF LASER EXHAUST EXTERNAL TO SPACECRAFT

Shaul Abramovich

November 1985

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The work reported herein was carried out for the Naval Postgraduate School by Dr. Shaul Abramovich under Contract Number N62271-83-M-1939. The work presented in this report is in support of DARPA project. The work is based on general publications and theory and provides specific means for solving the exhaust flow from a spacecraft laser. Computer programs have been developed to calculate the flowfield in the continuum region as well as in the molecular region. It provides the means to calculate the flux of the exhausted gas towards the walls of the spacecraft. The project on LASER EXHAUST is funded by Defense Advanced Research Projects Agency and is under the cognizance of Distinguished Professor A. E. Fuhs.

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20. Abstract (continued)

The continuum methods may be used as far as the limit where translational equilibrium ceases to exist. The breakdown of the continuum theory may be evaluated using the experimental breakdown parameter, as proposed by G. A. Bird. Beyond this limit, the molecular Direct-Simulation-Monte-Carlo method (DSMC) is applied.

The axisymmetric Monte Carlo Simulation begins outside the nozzle, where the breakdown parameter has a value of approximately 0.05. The actual shape of this breakdown limit is a closed lobe surface which starts at the nozzle lips, approximately follows a specific Mach wave in the Prandtl-Meyer fan and closes back to the axis far downstream. Because our interest is limited to the close vicinity of the corners, the shape of this limit may be approximated to a straight line (for an axisymmetric flow making a cone).

For the simulation purposes, the domain between the breakdown limit and the wall is divided into sectors, each sector divided into radial regions and each region into simulation cells. Each cell is filled with a number of simulated molecules relative to the cell volume and local number density.

The simulation is performed for each region separately and contains:

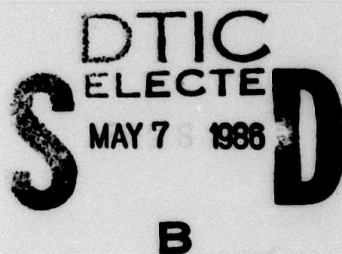
- * molecular motions
- * generation of new molecules to simulate input flows
- * deactivation of molecules to simulate output flows
- * molecular collisions

Because there is no apriori information about the flow interaction between different regions, the whole simulation is done on an iterative basis. A first run will supply the output flux from each region. These results are used as input data for consecutive runs.

The program runs as far as the collision frequency is still high and the mean free path is low compared with the size of the cells. Beyond this limit the flow may be regarded as collisionless, and the flux towards the solid wall may be computed directly.

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ABSTRACT

Some procedures have been developed to analyze the flowfield of highly underexpanded axisymmetric ring jets operated at high altitudes. The Method of Characteristics (MOC) was used to compute the Prandtl-Meyer expansion fan and the flow parameters in that region. The MOC may also be used to obtain some indications about the repetitive expansion — compression behavior of the jet as well as the divergent shape of the expansion part downstream, when the ambient pressure goes below certain limits.

The continuum methods may be used as far as the limit where translational equilibrium ceases to exist. The breakdown of the continuum theory may be evaluated using the experimental breakdown parameter as proposed by G. A. Bird. Beyond this limit, the molecular Direct-Simulation-Monte-Carlo method (DSMC) is applied.

The axisymmetric Monte Carlo Simulation begins outside the nozzle, where the breakdown parameter has a value of approximately 0.05. The actual shape of this breakdown limit is a closed lobe surface which starts at the nozzle lips, approximately follows a specific Mach wave in the Prandtl-Meyer fan and closes back to the axis far downstream. Because our interest is limited to the close vicinity of the corners, there the shape of this surface may be approximated by a straight line (making a cone in an axisymmetric flow).

For the simulation purposes, the domain between the breakdown surface and the wall is divided into sectors, each sector divided into radial regions and each region into simulation cells. Each cell is filled with a number of simulated molecules relative to the cell volume and local number density.

The simulation is performed for each region separately and contains:

- * molecular motions
- * generation of new molecules to simulate input flows
- * deactivation of molecules to simulate output flows
- * molecular collisions

Because there is no apriori information about the flow interaction between different regions, the whole simulation is done on an iterative basis. A first run will supply the output flux from each region. These results are used as input data for consecutive runs.

The program runs as far as the collision frequency is still high and the mean free path is low compared with the size of the cells. Beyond this limit the flow may be regarded as collisionless, and the flux towards the solid wall may be computed directly.

I. INTRODUCTION

Gas jets released from spacecrafts and external flows about vehicles at high altitudes have a renewed interest in particular with regard to two main aspects:

- a. contamination of the spacecraft walls
- b. optical disturbances caused by the plume.

A spacecraft gas dynamics laser releasing a large quantity of gas is highly affected by these two factors and the interest in analyzing them and being able to control them have a unique importance in further development.

A spacecraft laser is assumed to have a long cylindrical shape with the optical power output devices installed at one of its bases as shown in Figure 1.

The output gas is released through a ring nozzle, undergoes a fast three dimensional axisymmetric expansion, and forms a plume covering the whole meridian plane of the vehicle. It widens to large angles of expansion so that it may intersect the laser beam. Back scattered molecules may return to the wall of the spacecraft causing contamination and degradation of surfaces and vehicle parts.

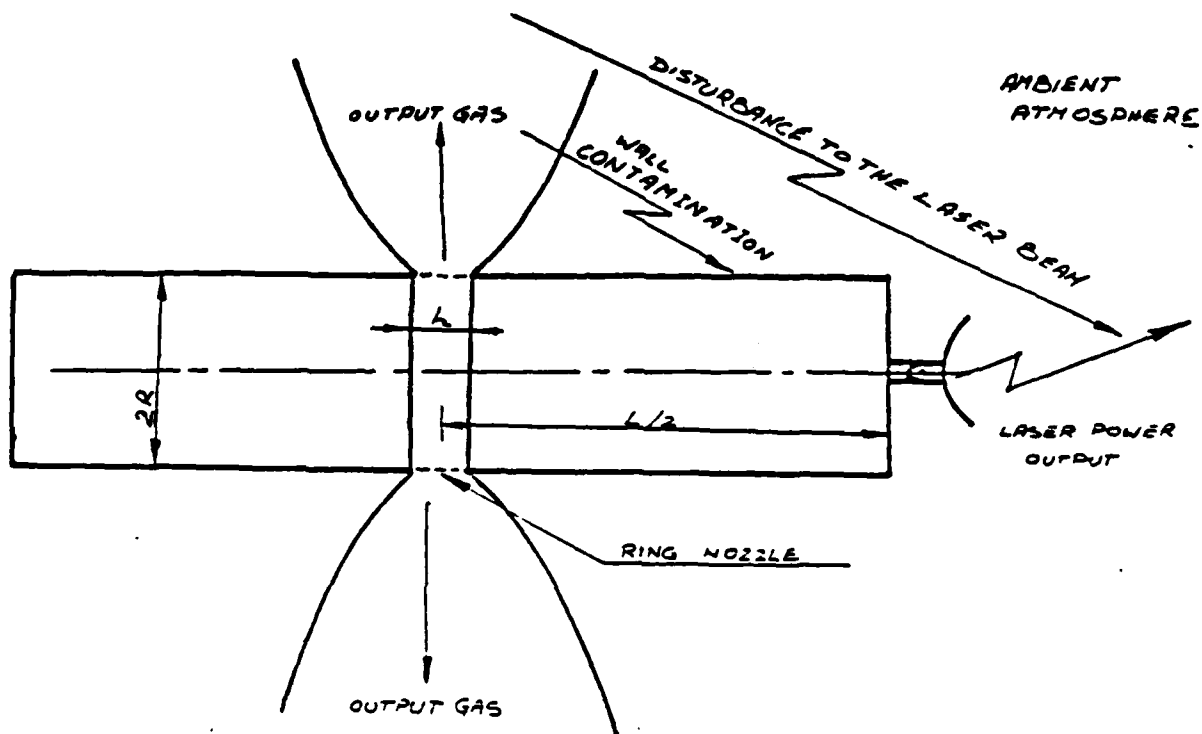


Figure 1. The Spacecraft Laser.

M_0 - Mach number at the exit surface ~ 4 the jet gas is composed of two species

heavy molecules $M_{G1} = 19$

light molecules $M_{G2} = 4$

Altitudes between 200 to 1000 km.

Continuum flow theory may be used to solve the flowfield and flow parameters as far as there is translational equilibrium, it means that intermolecular interactions are fast enough to maintain expansion rates. Wherever these interactions are too slow, the continuum flow becomes invalid and the molecular flow theory should be employed.

The solution for the continuum regime is computed here by means of the Method of Characteristics (MOC) [1,2,3]. The limit where continuum breakdown occurs was estimated by the experimental breakdown parameter as proposed by G. A. Bird [4]. Beyond this limit, it is proposed to compute the molecular flow by means of the Direct Simulation Monte Carlo technique as described in detail by Bird [4].

For moderate and low pressure ratios (static pressure at the nozzle exit to the ambient pressure), an underexpanded jet exhibits a repetitive expansion - compression behavior with a geometry depending on the initial Mach angle, on the Prandtl-Meyer fan angle, and on the gas specific heats ratio. For lower ambient pressure which occurs at higher altitudes, the first compression region is pushed out to the envelope of the jet forming the barrel shock. If the ambient pressure is low enough, this compression region may disappear due to the molecular behavior of the flow [6,11].

The breakdown of the continuum theory occurs in a region where the gas density and pressure are high compared with the density and pressure in the ambient gas. At high altitudes the ratios between these parameters may reach 10^6 or more. Considering this range of variations, computational validity dictates the use of the Direct Simulation Monte Carlo method. In the higher density range the jet will be considered as consisting of two species of gas, their molecular model will be "the hard sphere molecule" model and

ambient gas is not allowed to protrude. In the lower density region the flow will be regarded as collisionless.

In the following chapters we bring the detailed description of the computer programs which solve the different parts of the flowfield.

II. THE CONTINUUM REGIME

A. THE TWO DIMENSIONAL ISENTROPIC UNDEREXPANDED JET

The results brought here are based on the supersonic steady isentropic flow theory as described in literature (see for example, Shapiro [1], Liepman and Roshko [2], and Owczarek [3]).

The ranges of parameters of a jet emerging from a gas dynamics spacecraft laser are:

a. The Mach number at the exit surface $M_0 = 4$. The static pressure at the exit plane $P_0 = 136\text{pa}$. Ambient pressure (P_{amb}), temperature (T_{amb}) and other thermodynamic properties of ambient gas depend on the altitude as shown in Table 1. The jet gas may consist of DF, HF, Helium and other species. In the programs we limit the composition to two species: Air and He. (The program allows changes in the composition and types of gas.)

b. The pressure ratio $\frac{P_0}{P_{\text{amb}}}$ for the minimum required altitude (200 km) assures that the jet is highly underexpanded (we show later the influence of this ratio on the shape of the jet).

The following thermodynamic relations are valid as long as the compressible flow is isentropic

$$T_T = T(1 + \frac{\gamma-1}{2} M^2) \quad (1)$$

$$P_T = P(1 + \frac{\gamma-1}{2} M^2)^{\frac{\gamma}{\gamma-1}} \quad (2)$$

$$\rho_T = \rho(1 + \frac{\gamma-1}{2} M^2)^{\frac{1}{\gamma-1}} \quad (3)$$

TABLE 1

ATMOSPHERIC DATA
(Abstracted from U.S. Standard Atmosphere 1976)

Altitude km	Pressure m bar	number density m ⁻³	particle speed m/sec	collision frequency sec ⁻¹	mean free path m	molecular weight kg/kmol	density kg/m ³	temperature °K
100	3.2011 -4	1.189 +19	381.4	2.68 +3	1.42 -1	28.4	5.604 -7	195.08
200	8.4736 -7	7.182 +15	921.6	3.9	2.4 +2	21.3	2.541 -10	854.56
300	8.7704 -8	6.509 +14	1079.7	4.2 -1	2.6 +3	17.73	1.916 -11	976.01
400	1.4518 -8	1.056 +14	1148.5	7.2 -2	1.6 +4	15.98	2.803 -12	995.83
500	3.0236 -9	2.192 +13	1215.0	1.6 -2	7.7 +4	14.33	5.215 -13	999.24
600	8.2130 -10	5.950 +12	1356.4	4.8 -3	2.8 +5	11.51	1.137 -13	999.85
700	3.1908 -10	2.311 +12	1627.0	2.2 -3	7.3 +5	8.00	3.070 -14	999.97
800	1.7036 -10	1.234 +12	1954.3	1.4 -3	1.4 +6	5.54	1.136 -14	999.99
900	1.0873 -10	7.876 +11	2192.6	1.0 -3	2.1 +6	4.40	5.759 -15	1000.00
1000	7.5138 -11	5.442 +11	2318.1	7.5 -4	3.1 +6	3.94	3.561 -15	1000.00

where T_T , P_T , and ρ_T are the total temperature, pressure and density (constant for isentropic field). T , P , and ρ are local temperature, pressure and density γ is the specific heat ratio of the gas (considered here as constant), M is the local Mach number.

The partial differential equation of motion for supersonic 2-D irrotational and isentropic flow is a hyperbolic equation having solutions obtained from invariants along characteristic lines. Physical interpretation of these lines are the compression or expansion waves which are oriented at Mach angles relative to the streamlines.

Once the directions of the characteristics (waves) are determined everywhere in the field, all other parameters may be calculated.

B. THE TWO DIMENSIONAL PLANAR JET

The compressible supersonic jet flow is characterized by two families of characteristics (pressure waves) starting at each corner of the nozzle lips. Each of these families of waves forms a Prandtl-Meyer fan. The streamlines crossing the characteristic waves bend outwards resulting in an increase in the flow area. The angle μ between the streamline and the pressure wave is a function of the local Mach number as

$$\mu = \arcsin (1/M) \quad (4)$$

The symbol μ is the Mach angle.

Using the isentropic relations, we can find the relation between the turning angle (θ) and the local Mach number (M) as

$$d\theta = - \frac{(M^2 - 1)}{M(1 + \frac{\gamma-1}{2} M^2)} dM \quad (5)$$

Integration between the conditions $M=1$ and M gives the total turning angle starting at the throat (where $M=1$) up to a point with given M . The result gives the Prandtl-Meyer function (angle) as

$$v(M) = \frac{\gamma+1}{\gamma-1} \arctg \frac{\gamma-1}{\gamma+1} (M^2-1) - \arctg (M^2-1) \quad (6)$$

In the close vicinity of the nozzle lips where the two families of characteristics do not intersect with each other there is a "simple region" of expansion. There the flow parameters are defined by v and θ of each characteristic line. Further downstream the waves intersect each other. In this part of the flow parameters are defined by the two intersecting characteristics. A singularity occurs when the initial Mach number is unity and a special treatment is required to start the calculations at that point (this special treatment has not been brought here). A particular importance of the Prandtl-Meyer function is when analyzing the two dimensional flow using the hodograph plane.

C. THE HODOGRAPH PLANE FOR A TWO DIMENSIONAL JET

The hodograph plane is a representation of the flow parameters in the velocity plane. Figure 2 shows a hodograph plane calculated for a simple gas ($\gamma=1.4$). The circles represent constant Mach numbers and constant

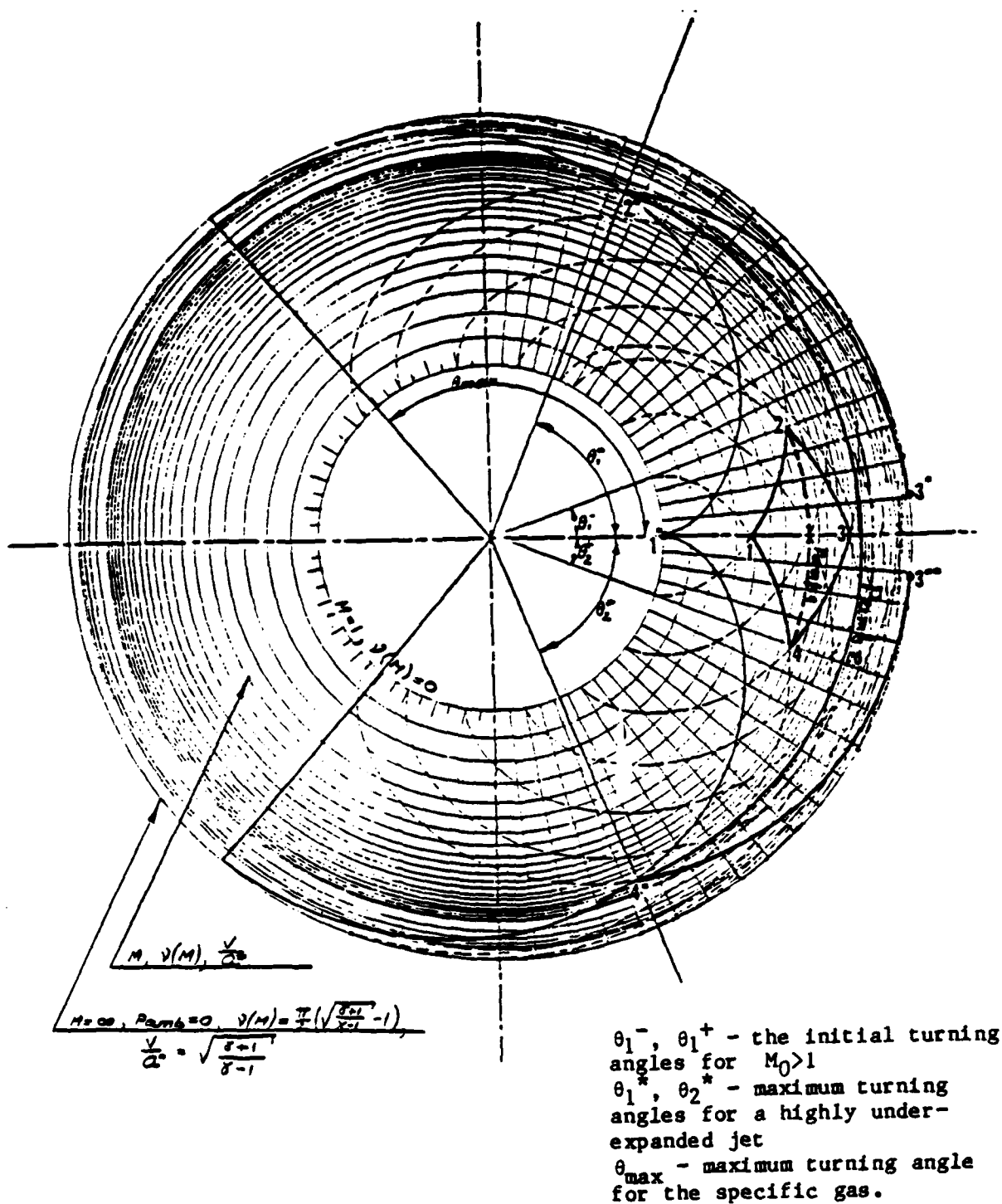


Figure 2. The Hodograph Plane.

1-2-3-4-1 defines a jet with $M_0 > 1$ expanding into $P_{amb1} < P_0$,
 resulting simple repetitive expansion-compression.
 1*-2*-3*-4*-1* defines a jet with $M_0 = 1$ expanding into
 $P_{amb2} \ll P_0$, resulting in a highly underexpanded jet.

pressure ratios $(\frac{P}{P_T})$. The epicycloids are the two families of characteristics. The angles θ are the turning angles due to expansion or compression (which are both present in supersonic jets).

To define an isentropic supersonic jet on the hodograph plane it is necessary to define the Mach number at the exit plane, the pressure ratios $(\frac{P}{P_T})$ and $(\frac{P_{amb}}{P_T})$, and the specific heat ratio (γ) of the gas.

Investigating the shapes of the jet as a function of ranges of parameters we may get:

- a. simple underexpanded jets for which $\frac{P_{amb}}{P_T}$ is high enough so that the two families of characteristics intersect each other.
- b. a critical underexpanded jet for which $\frac{P_{amb}}{P_T}$ is low enough so that the intersection between the outer characteristic lines of the two families occur on the outer hodograph circle.
- c. highly underexpanded jets for which a part of characteristics do not intersect at all.
- d. expansion into complete vacuum so that there are no reflections from the jet boundaries and therefore the compression region disappears.

D. THE SHAPES OF TWO DIMENSIONAL JETS

The following paragraphs further detail the different shapes.

1. Simple Underexpanded Jets

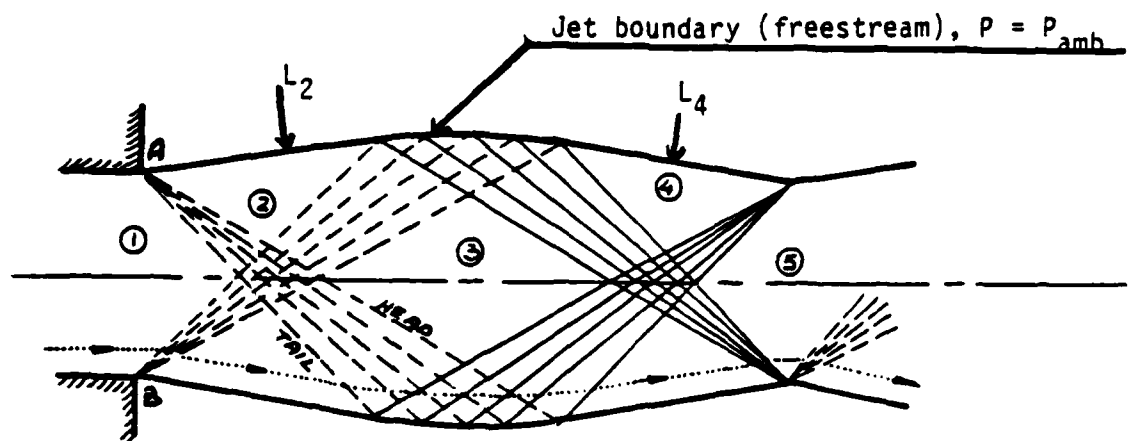
Figure 3 shows the physical plane and the hodograph plane of a simple underexpanded jet. If $M_0 > 1$, an initial turn of the flow θ_0 is made within the nozzle. An additional turn of θ is due to the underexpansion. θ is found by the intersection of characteristics (1-2) with the circle defined by P_{amb}/P_T .

When $M_0 > 1$, the characteristic line 1-2 is described in the physical plane by a region in which only one family of expansion waves are present (simple region, see transverse line between 1 to 2 in the physical plane). A different family of expansion waves forms a second simple region when moving between 2 to 3. At a larger distance from the exit plane, reflected waves from the free streamline (jet boundary) cause compression. An ideal representation of such a jet is a repetitive pattern of expansion and compression.

For $M_0 = 1$, the tail waves of both families are perpendicular to the flow, thus, both lie on line AB. That means that if $M_0 = 1$ there is no simple region near the exit plane of the jet. The characteristic line 1-2 on the hodograph plane becomes a single point A (or B) when located in the physical plane.

2. Critical Underexpanded Jets

We define a critical underexpanded jet when point (3) (see Figure 4) lies on the limiting circle M_∞ or $P/P_\infty = 0$. This means that there is a core within the jet where the pressure approaches zero and Mach approaches infinity. This core is theoretically bounded at its upstream side by expansion waves and downstream by compression waves.



——— compression waves
 - - - expansion waves
 streamline

- ① uniform axial flow ($P=P_0$)
- ② uniform flow parallel to L_2 ($P=P_{amb}$)
- ③ uniform axial flow (lowest pressure- P_{min})
- ④ uniform flow parallel to L_4 ($P=P_{amb}$)
- ⑤ uniform axial flow ($P=P_0$)

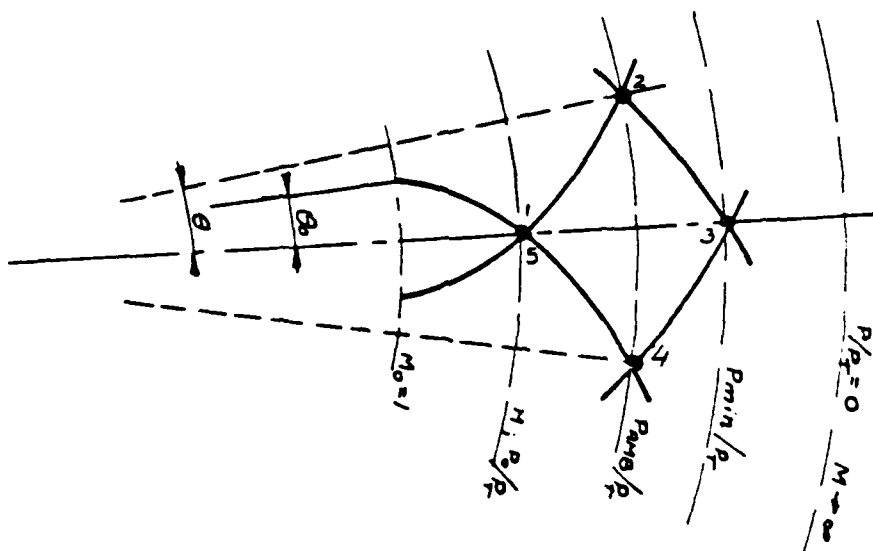


Figure 3. Flow at exit of a simple underexpanded jet.

- (a) physical Plane
- (b) Hodograph Plane

Using the theoretical expressions for isentropic ideal flow one may derive the values of $\frac{P_{amb}}{P_T}$ or $\frac{P_{amb}}{P_o}$ as function of M_o which causes a jet to be critical underexpanded.

Figure 5 shows results of $\frac{P_{amb}}{P_o}$ as functions of M_o for gases with different specific heat ratio.

3. Highly Underexpanded Jets

When P_{amb} is lower than the critical values as shown in figure 4, point 3 does not exist (there is no intersection between lines 2-3 2'-3'). This means that the repetitive reversible expansion/compression shapes ceases to exist. The envelope of the jet starts at an angle defined by θ at the nozzle exit plane and approaches an asymptotic angle defined by θ_{lim} (see Figure 6).

In this case we get two (symmetric) groups of characteristics C_1 - C_2 and C'_1 - C'_2 (Figure 6) with no intersection between them. C_1 and C'_1 define the inner limit for reflected characteristics, C_2 and C'_2 define the outer limit. As the rest of reflected waves lie between C_2 or C'_2 and the jet boundary, we may conclude that a compression region may exist only in a layer along the jet boundary.

Because of irreversible effects such as shear stresses, heat transfer due to high temperature gradients, or condensation effects in real gases, the compression layer may be interpreted as the "barrel shock".

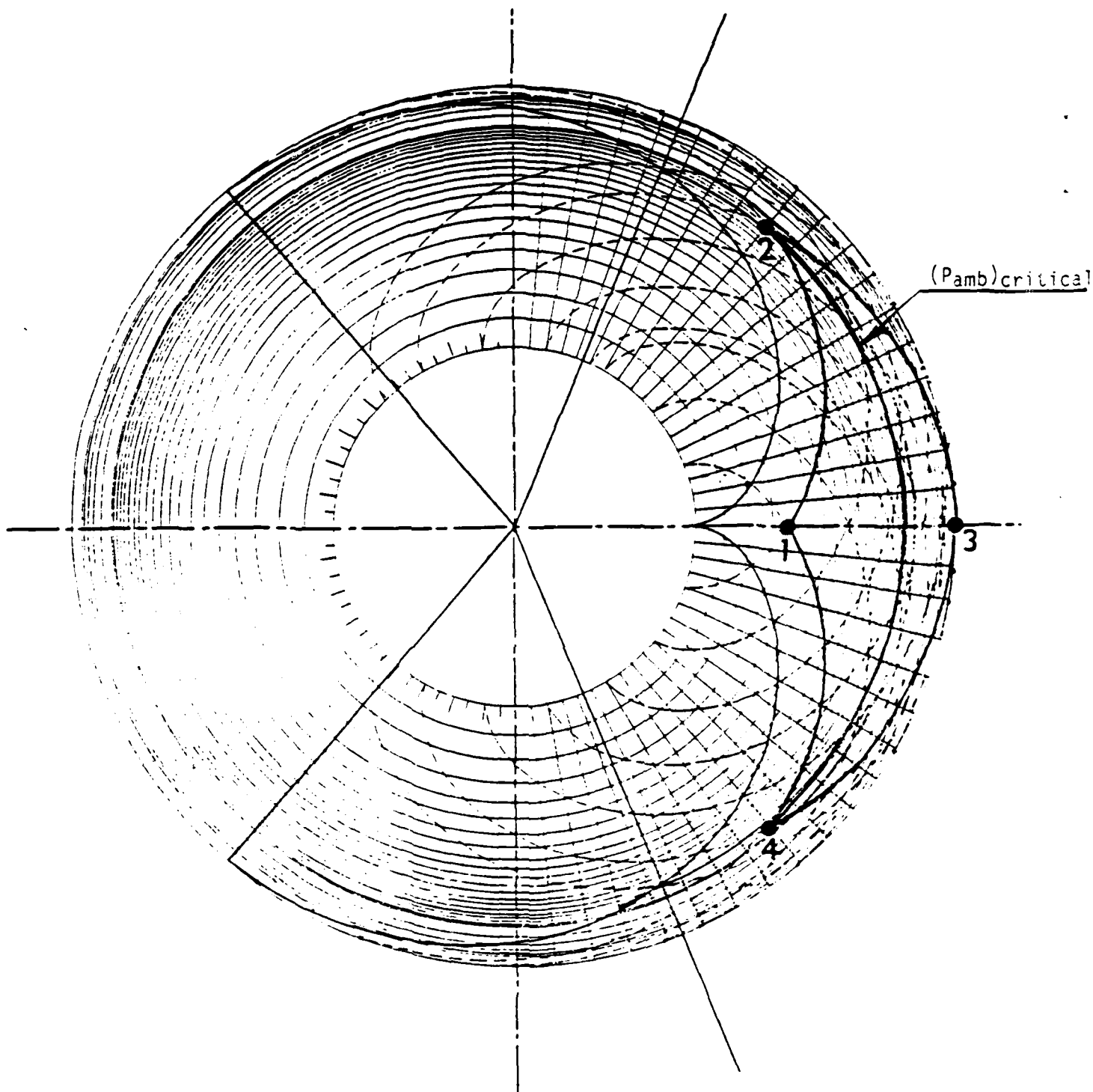


Figure 4. The Hodograph Plane for a Critical Underexpanded Jet.

(1-2-3-4-1), ($\gamma=1.4$)

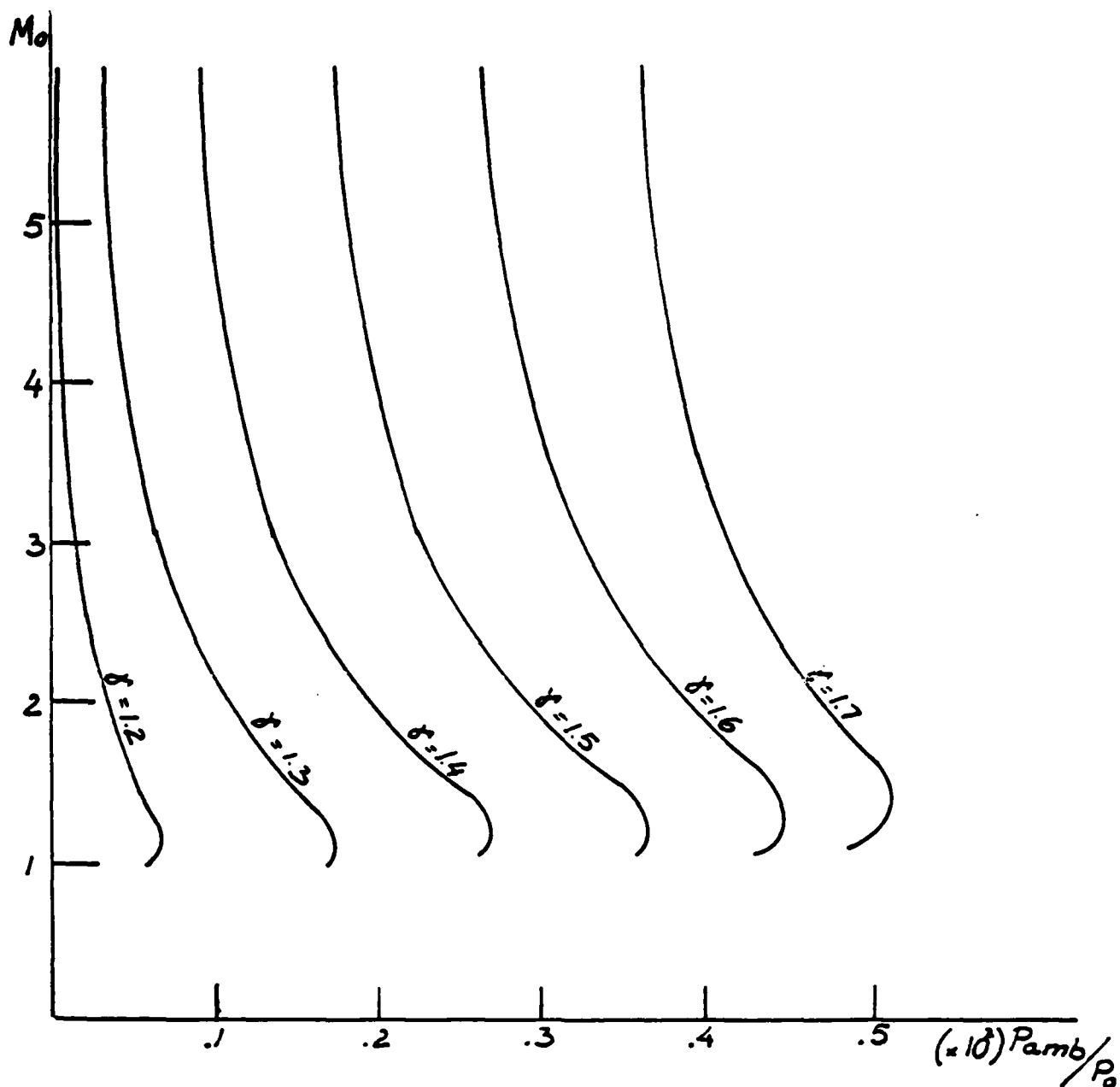


Figure 5. Dependence of critical values of P_{amb}/P_0 on the Mach number at the exit plane (M_0) for different values of specific heat ratio (γ).

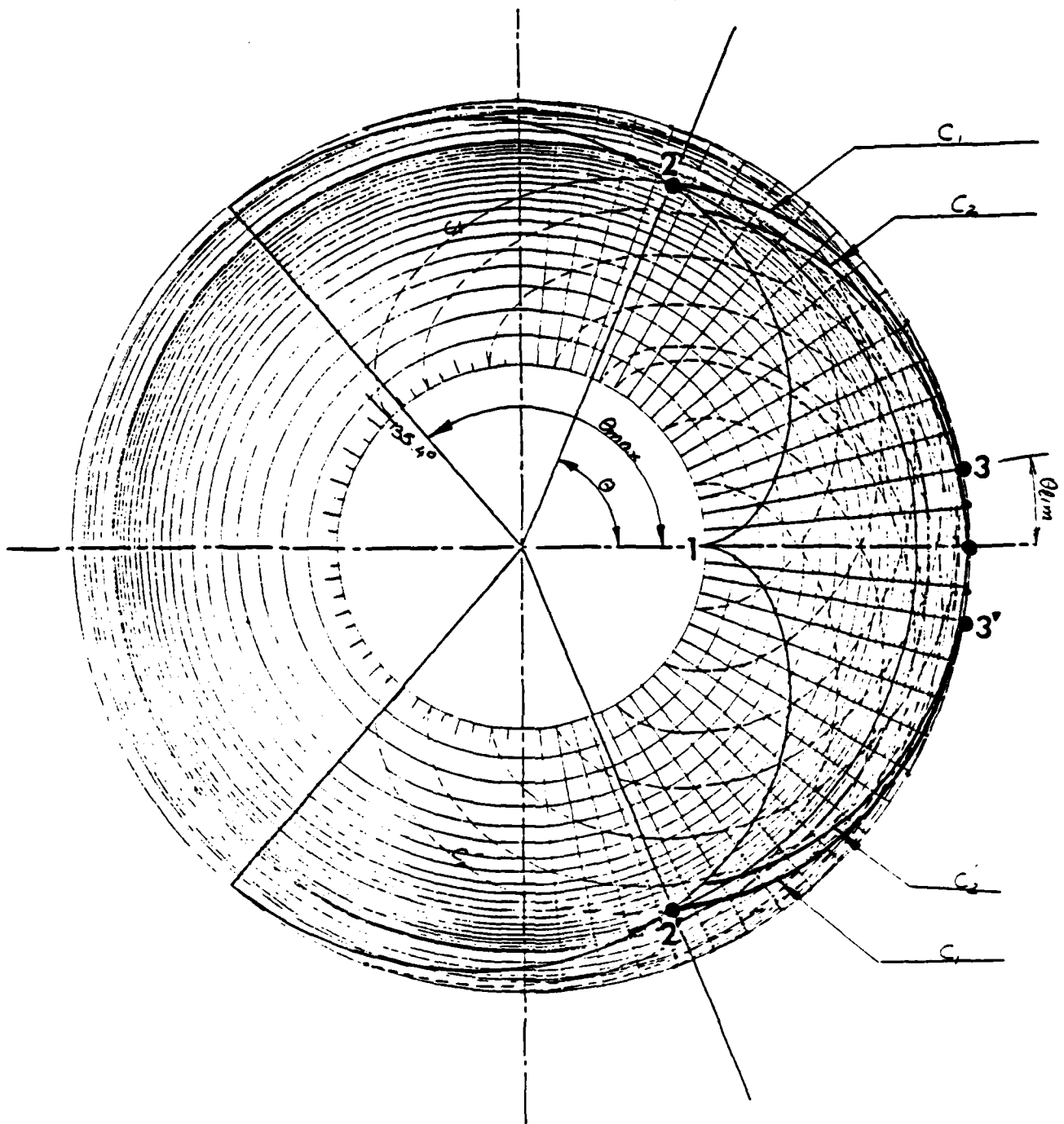


Figure 6. The Hodograph Plane for a Highly Underexpanded Jet

($\gamma = 1.4$)

θ_{\max} - maximum turning angle

θ - total turning angle in the specific jet $\theta > \theta_{\max}/2$

θ_{\lim} - limiting angle of compression region.

Figure (7) shows the hodograph plane for an air jet ($\gamma=1.4$) expanding into an ambient pressure 105 times lower than the static pressure at the exit plane. Figure (8) is a schematic description of the jet (the data for this jet is given in Table 2). The shape shown in Figure (8) may be compared with the barrel shock photograph in page 208 Reference [3].

4. EXPANSION INTO A COMPLETE VACUUM - $P_{amb}=0$

This is an extreme situation in which the maximum turn angle of streamlines occur near the nozzle exit plane. The theoretical free stream is defined only by the theoretical turning angles. All streamlines in the flow expanded monotonically towards $P=0$ without being reflected by the jet boundaries.

TABLE 2

CALCULATION OF CHARACTERISTICS ON PHYSICAL PLANE

State	θ_* +	θ_* -	θ	$v(M)$	M	μ	$\theta + \mu$	$\theta - \mu$	P/P_t
1	0	0	0	0	1	90°	90°	-90°	0.5283
2	0	10	10	10	1.435	44.15	54.15	-34.15	
3	0	20	20	20	1.775	34.3	54.3	-14.3	.2990
4	0	40	30	30	2.135	27.93	57.93	2.07	.1810
5	0	60	40	40	2.54	23.18	63.18	16.82	.1035
6	0	80	50	50	3.013	19.38	69.38	30.62	.55 -1
7	0	100	60	60	3.595	16.15	76.15	43.85	.2672 -1
8	0	120	67.7	67.7	4.145	13.96	88.7	53.74	.1146 -1
9	20	135.4	0	20	1.775	34.3	34.3	-34.3	.5437 -2
10	20	20	10	30	2.135	27.93	37.93	-17.93	.1810
11	20	40	20	40	2.54	23.18	43.18	- 3.18	.135
12	20	60	30	50	3.013	19.38	49.38	10.62	.55 -1
13	20	80	40	60	3.595	16.15	56.15	23.85	.2672 -1
14	20	100	50	70	4.339	13.315	63.32	36.69	.1146 -1
15	20	120	57.7	77.7	5.085	11.34	69.04	46.4	.425 -2
16	40	135.4	0	40	2.54	23.18	23.18	-23.18	
17	40	40	10	50	3.013	19.38	29.38	- 9.38	.55 -1
18	40	60	20	60	3.595	16.15	36.15	3.85	.2672 -1
19	40	80	30	70	4.339	13.315	43.32	16.69	.1146 -1
20	40	120	40	80	5.3479	10.777	50.78	29.23	.4215 -2
21	40	135.4°	47.7	87.7	6.433	8.943	56.64	38.76	
22	60	60	0	60	3.595	16.15	16.15	-16.15	.1146 -1
23	60	80	10	70	4.339	13.315	23.32	- 3.32	.4215 -2
24	60	100	20	80	5.3479	10.777	30.78	9.22	
25	60	120	30	90	6.8190	8.433	38.43	21.57	
26	60	135.4°	37.7	97.7	9.2105	6.2330	43.93	31.5	
27	80	80	0	80	5.3479	10.777	10.777	-10.77	
28	80	100	10	90	6.8190	8.433	18.433	1.57	
29	80	120	20	100	9.2105	6.233	26.23	13.8	
30	80	135.4	27.7	107.7	12.45	4.61	32.3	23.1	
31	100	100	0	100	9.2105	6.233	+ 6.233	- 6.233	
32	100	120	10	110	13.874	4.1331	14.13	5.9	
33	100	135.4	17.7	117.7	21.4	2.678	20.37	15.0	
34	120	120	0	120	27.335	2.097	2.097	- 2.097	
35	120	135.4	7.7	127.7	104	0.546	8.2	7.2	
36	-	-	11°	-	-	0	-	-	0
51	20	115.4	47.7	67.7°	4.145	13.96		33.7	.5437 -2
52	40	115.4	37.7	77.7	5.085	11.34		26.36	
53	40	95.4	+27.7	67.7°	4.145	13.96		13.7	.5437 -2
54	60	75.4	+ 7.7	67.7°	4.145	13.96		- 6.26	.5437 -2
55	60	95.4	17.7	77.7	5.085	11.34		6.4	
56	60	115.4	27.7	87.7	6.433	8.943		18.8	

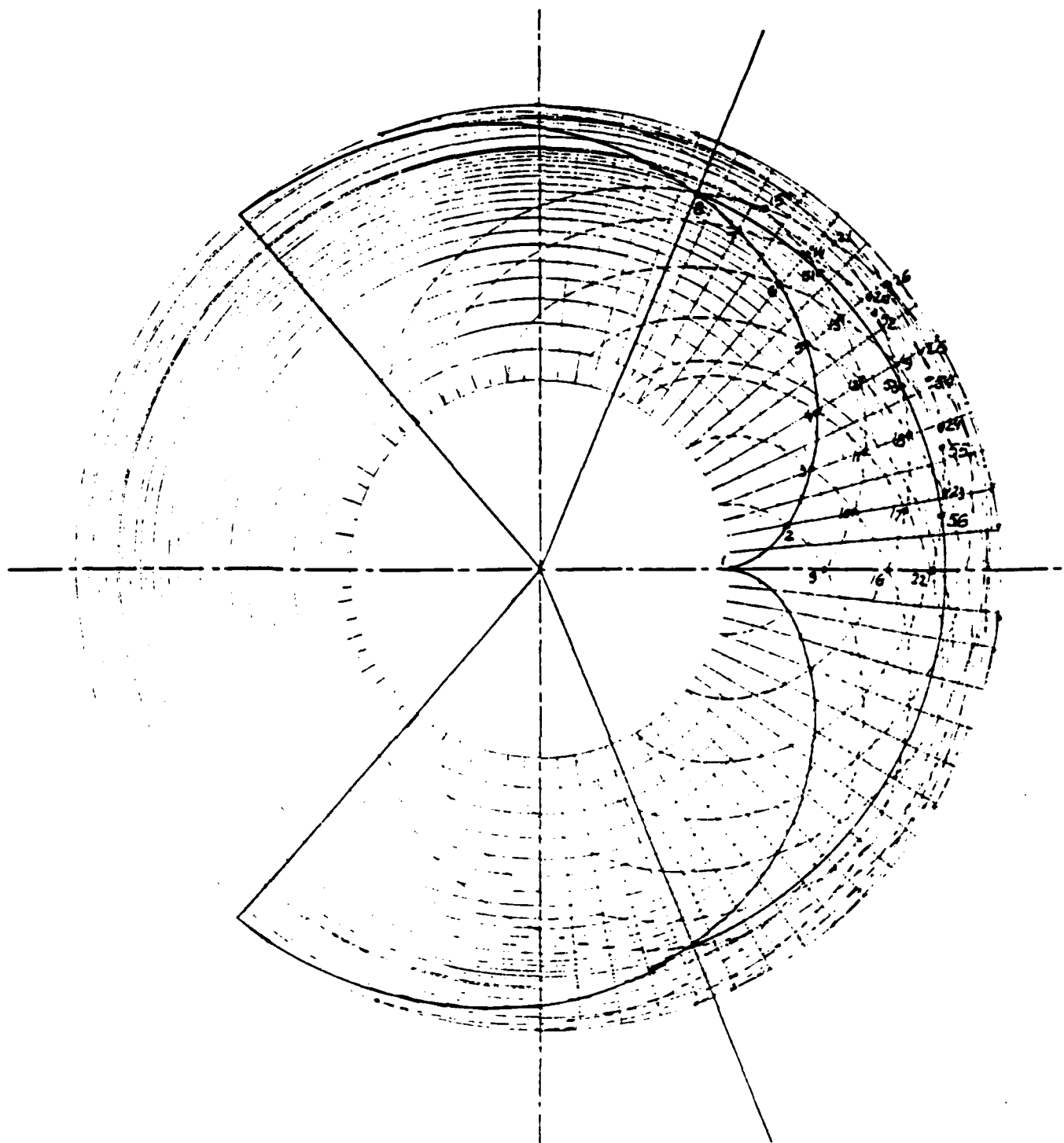


Figure 7. Hodograph plane showing the points on the mesh of characteristics.
(Related to physical plan Figure 8).

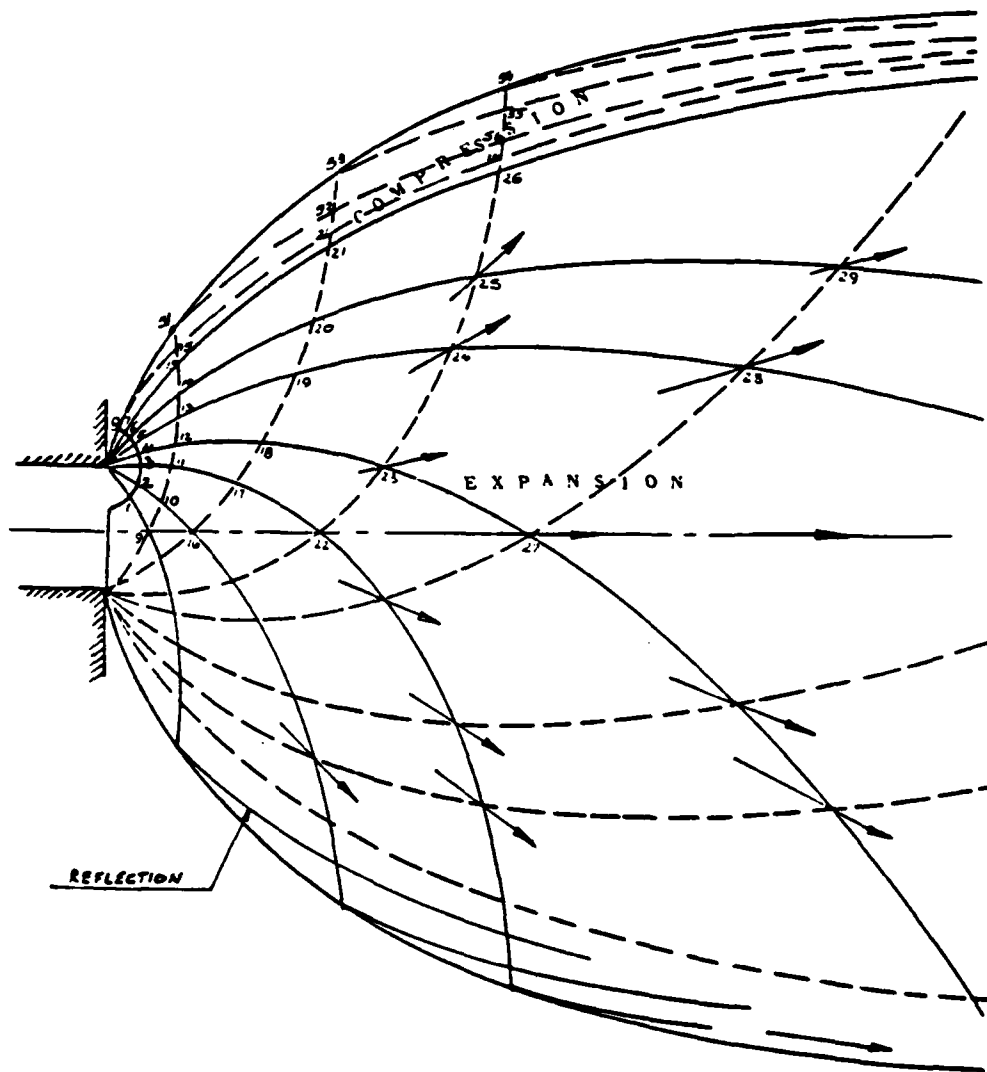


Figure 8. Schematic shape of a highly underexpanded jet.

(See Figure 7 - The Hodograph Plane)

The arrows indicate flow direction.

E. THE METHOD OF CHARACTERISTICS; COMPUTATION OF PLANAR AND AXISYMMETRIC TWO-DIMENSIONAL FLOWS

For a planar two dimensional flow, the Prandtl-Meyer function v and flow direction θ at any point (3) in the field may be calculated using data of two other points (1) and (2) located on characteristic lines that intersect at (3) (see Fig. (9))

$$v_3 = \frac{1}{2} (v_1 + v_2) + \frac{1}{2} (\theta_1 - \theta_2) \quad (7)$$

$$\theta_3 = \frac{1}{2} (v_1 - v_2) + \frac{1}{2} (\theta_1 + \theta_2) \quad (8)$$

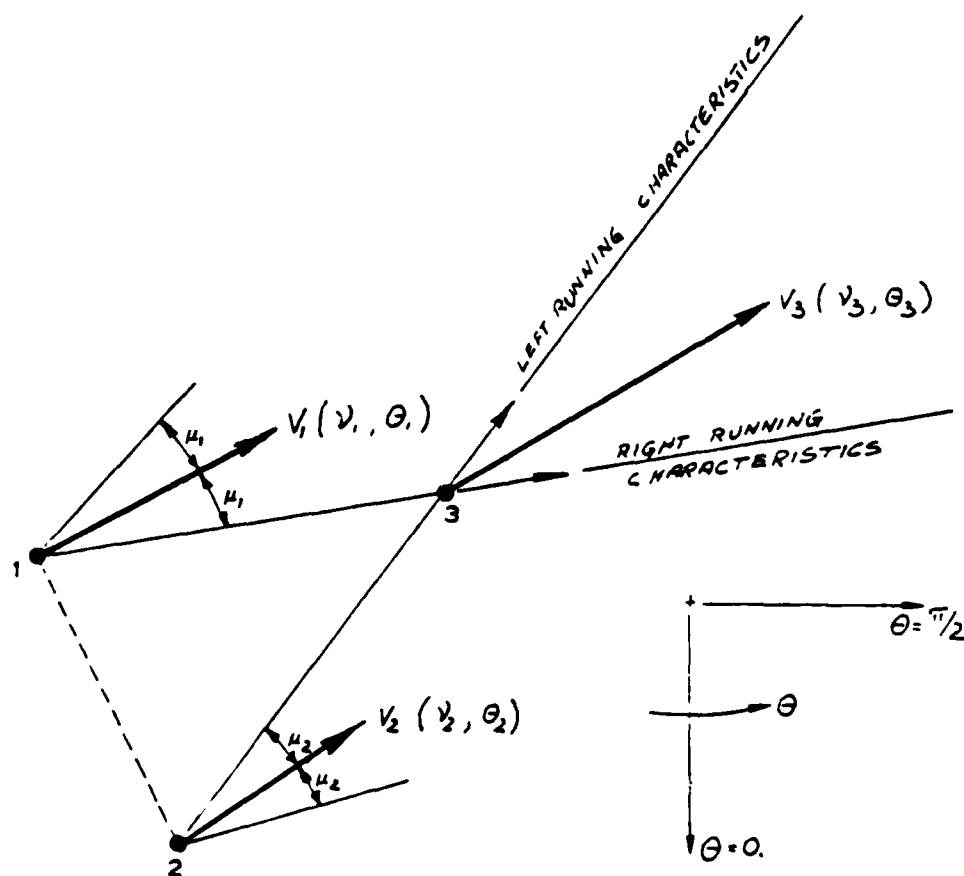


Figure 9. The calculation of v and θ for point (3) is based on data for points 1 and 2.

For axisymmetric, two-dimensional flow, Liepmann and Roshko [2] developed expressions for finding the Prandtl-Meyer function (v) and the flow direction (θ) which are given by:

$$v_3 = \frac{1}{2} (v_1 + v_2) + \frac{1}{2} (\theta_1 - \theta_2) + \frac{1}{2} \left[\sin \mu_1 \frac{\sin \theta_1}{r_1} \Delta \xi_{13} + \sin \mu_2 \frac{\sin \theta_2}{r_2} \Delta \eta_{23} \right] \quad (9)$$

$$\theta_3 = \frac{1}{2} (v_1 - v_2) + \frac{1}{2} (\theta_1 + \theta_2) + \frac{1}{2} \left[\sin \mu_1 \frac{\sin \theta_1}{r_1} \Delta \xi_{13} - \sin \mu_2 \frac{\sin \theta_2}{r_2} \Delta \eta_{23} \right] \quad (10)$$

The angles and subscripts are shown in Figure (10).

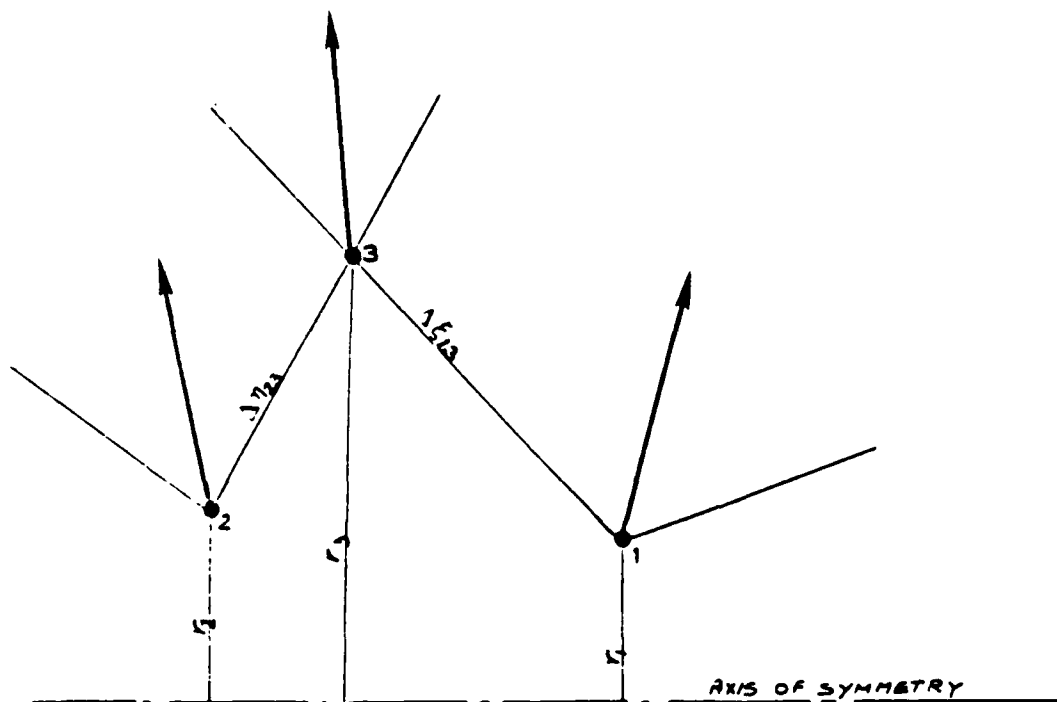


Figure 10. Calculation of θ and v for axisymmetric flow.

It is obvious that for the axially symmetric flows the increase in the radius causes the increase in the flow cross section and influences the flow direction and the Prandtl-Meyer function. These facts have been taken into account when developing the "compatibility equations" (9,10).

Using equations (9,10) we have developed a computer program which enables the calculation of the jet flow for a two dimensional and for an axially symmetric geometry (ring jet).

The listing of the program, the program description and some results are given in Appendix A.

III. THE BREAKDOWN OF THE CONTINUUM THEORY

A. GENERAL CRITERIA

As described in detail by Bird (Chapter 1 Reference [4]), the validity of the continuum approach has been identified with the validity of the Navier Stokes equations. This requires that the Knudsen number $K_n = \lambda/L$ should be small compared with unity (λ is the mean free path and L is a scale length for the specific flow field). For K_n larger than a certain limit (between 0.01 to 0.1 depending on the required accuracy) a microscopic approach is necessary.

For small values of L , the microscopic approach may lead to statistical fluctuations of the results due to the small number of molecules participating in the flow processes. In figure (11) which was reproduced from Bird's book [4, figure 1.6], the regimes of rarefied flow and high fluctuations are depicted. The flow around the jet-air boundaries near a spacecraft is generally rarefied (high Knudsen number), but has insignificant fluctuations.

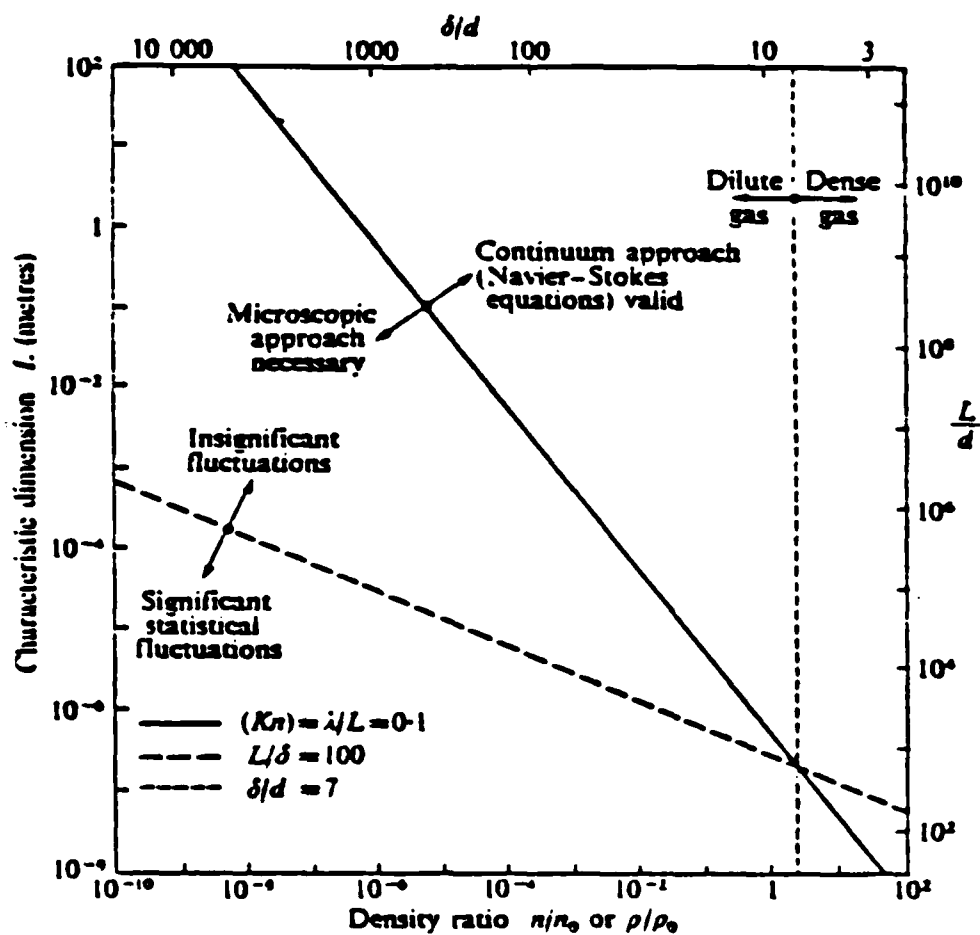


Figure 11. Limits for continuum approach and microscopic approach ($d=3.7 \times 10^{-10}$ m).

B. THE EMPIRICAL CRITERION

The Method of Characteristics (MOC) was used to compute the jet flow and the results obtained from the computer program "AXSYM" are valid as long as the continuum flow theory is valid.

The continuum flow requires that the mean free path should be negligibly small in comparison with the scale length of the macroscopic flow variations. The classical theory for Prandtl-Meyer expansion may therefore be expected to fail at progressively larger distances from the nozzle lips as the gas density decreases with the increasing flow angle and Mach number. The empirical criterion for the breakdown of continuum flow in steady expansion flow [4] is that

$$P \equiv \frac{q}{\rho v} \left| \frac{d\rho}{dS} \right| \approx 0.05 \quad (11)$$

where

q = stream velocity

ρ = density

v = molecular collision frequency

$\left| \frac{d\rho}{dS} \right|$ = absolute change in density while moving a distance
 dS along a streamline

Introducing the breakdown parameter P into the program, gives the definition of the boundary where the flow should be calculated by means of the molecular flow theory, i.e., by solving the Boltzmann equation.

For an underexpanded jet with a high initial Mach number, the breakdown surface is nearly a streamline. Furthermore, the range of flow parameters for the present problem are such that the simple region extends to very large distances and near the nozzle lip the breakdown limit may be approximated by a straight line.

For the axisymmetric jet there is no simple region, however, for the region of interest it may be regarded as linear.

The method proposed in the present work for solving the flow behind the breakdown boundary is the Direct Simulation Monte Carlo (DSMC). For this purpose, a computer program "SIMUL" was developed. In the following chapter we describe the algorithms required for the specific problem, the geometry and the data organization. Detailed program description is given in Appendix (B).

IV. THE MOLECULAR FLOW IN AN AXISYMMETRIC RING JET

A. GENERAL CONSIDERATIONS

The part of the field in which the jet may be calculated by means of the continuum theory was described in Chapter II. There we calculated also the boundaries where continuum theory becomes invalid and molecular calculation should be employed. In fact, the molecular theory and the molecular Boltzmann equations are universal and hold for the entire flowfield. However, computational requirements make the Boltzmann equation impractical for the upstream flows. Therefore we limit our solution only to the part of the flow beyond the region where continuum breakdown occurs.

As a result obtained from MOC solution the "breakdown", i.e., the locus where the breakdown parameter p has values between 0.03 to 0.06, for the region close to the nozzle lips this boundary may be approximated by a straight line (for axisymmetric flow this line is the envelope of a cone, see Figure (12)).

For the specific jet and gas, the breakdown occurs in a region where the number density is in a range of 10^{21} molecules/m³. For ambient gas at an altitude of 200 km the number density is 10^{15} and decreases to a range of 10^{11} at 1000 km. In order to be able to express this vast change in a simulation, we would need to have an extremely large number of cells which would be impossible to store in a computer. To overcome this problem we are required to make a less exact formulation which enables the production of results, having to pay the penalty of "smearing" the steep gradients and obtaining averages within layers of simulated cells. Unfortunately it is impossible to

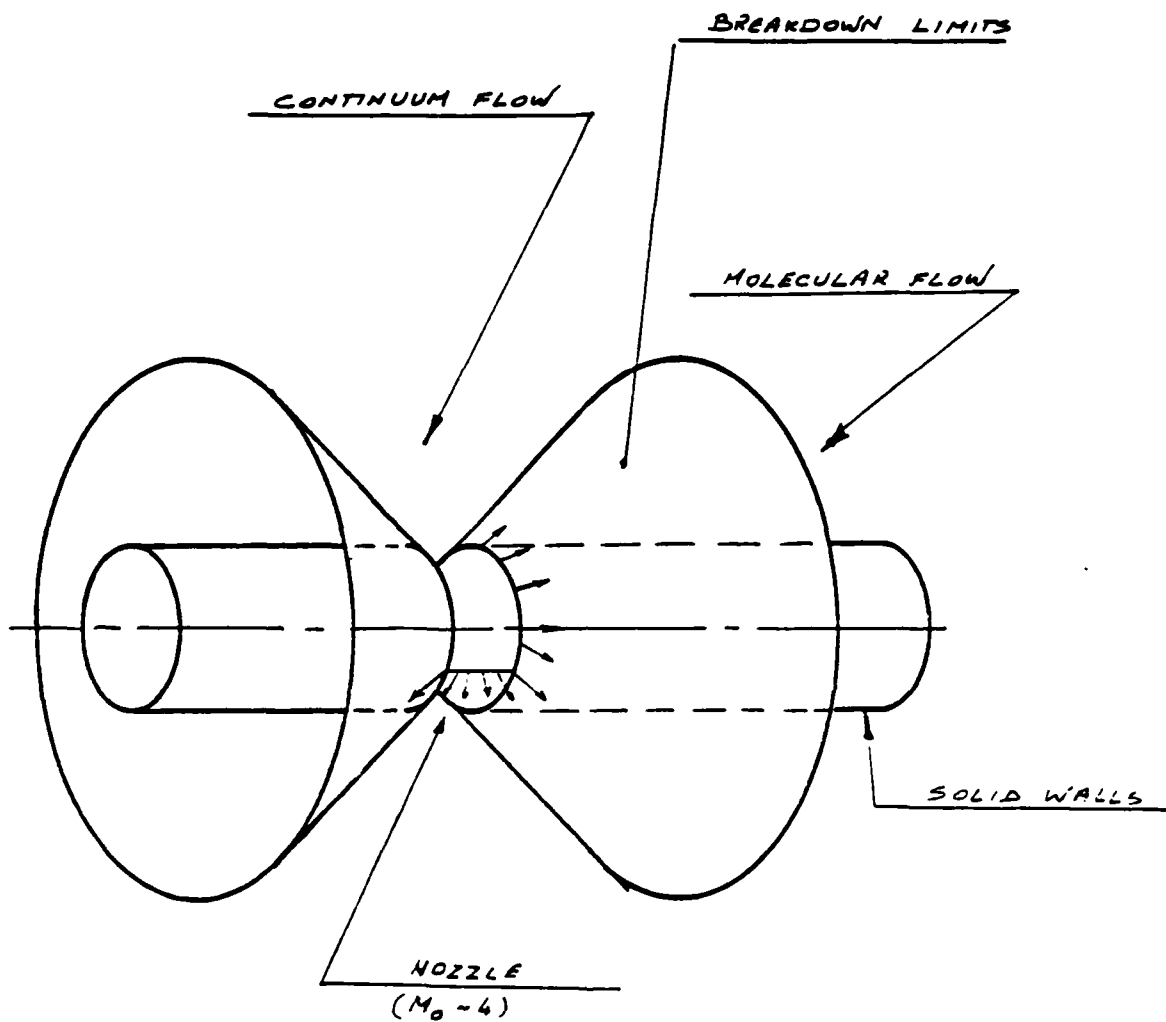


Figure 12. Regions in a ring jet.

predict how far the simulated results will be from the exact solutions. These comparisons have to be made after getting final results of this simulation.

1. The Direct Simulation Monte Carlo Method

The direct simulation Monte Carlo Method is a technique for a computer modeling of a real gas by some thousands of simulated molecules. The velocity components and the coordinates of the simulated molecules are stored in the computer and are modified with time as a result of collisions and boundary interactions. A detailed description of some problems and their solutions by means of direct simulation is given in [4].

To follow the molecular motion it is necessary to divide the simulated domain into a network of cells. The size of a cell must be such that the change in flow properties across each cell is small. The time is advanced in discrete steps DTM, such that DTM is small compared with the mean collision time per molecule. If there is a flow going through the domain, DTM should be small compared with the mean time required for the mean flow to cross the cells.* Both cell size ((DR),(DDALFA) - radial size and angular size as they appear in the program) and DTM may vary in the simulation with position and time.

Applications such as free jet expansion in which large gradients of flow properties are expected, may require a very large number of cells for the simulation. In these cases the computer memory requirements to store cells' data and molecules' data may exceed the available computer storage. A

*If DTM is chosen to be very small compared with the mean time between collisions then the simulation will require a very large number of runs such that the number of collisions will be sufficient. If DTM is large the molecules are washed out by the mean flux and there is no time for the collisions to influence the flow.

solution for this problem is to divide the simulation space into smaller regions and to run the simulation for each region separately. If there is an interaction between different regions, which a priori is undefined, the solution should be found iteratively. (That means that each run will provide data for consecutive runs and the procedure should be repeated until the results converge to a steady solution.

The computation of a representative set of collisions based on mean collision time per molecule is invalid for a computerized simulation because of the large computer time and computer memory requirements. Instead, the method proposed by Derzko which is described in details by Bird [4] may be employed. Following this method, an averaged mean time between collisions of species L with species M for a cell is calculated. The number of collisions of each type (L.M species) is such that the collision time counters are kept concurrent with the overall time parameter. The L.M collision time for a cell containing N_L and N_M molecules with collision cross section σ_{LM} , number densities n_L and n_M and relative velocity C_r , is given by

$$\Delta t_c = \frac{LP}{N_L} \frac{1}{\sigma_{LM} n_M C_r} + \frac{MP}{N_M} \frac{1}{\sigma_{LM} n_L C_r} \quad (12)$$

where LP and MP are the probabilities that the collision will be effective for the L and M molecules respectively.

B. THE GEOMETRY OF THE SIMULATED DOMAIN, SECTORS, REGIONS AND CELLS

Figure (13) shows a cross section of the simulated domain for the axisymmetric (ring) flow. Points A and A' are the nozzle lips. Starting at "A" and assuming the "breakdown" boundary to be a straight line, we obtain the cross section of the molecular domain as a sector defined by LAM. The solid wall is defined by AL. The arc LM may be assumed to be far enough so that the pressure along it may be assumed to equal the ambient pressure. Molecules originated in the jet cross the breakdown boundary with a velocity, direction, temperature (and other thermodynamic properties) as found from the continuum solution.

The molecular domain LAM is divided into secondary sectors, and each of these are divided into several radial regions making the "simulation regions".

Because we have no apriori information on how the expansion occurs, the angle of each sector (which mainly is in the direction of the expansion gradients) is left to be a result of the internal calculation.

Each region is divided into NRD radial divisions and NAD angular divisions making a network of $NAD \times NRD$ simulation cells. The angle DALFA of all regions in a sector is constant. Taking NAD constant for all regions in a sector, we get the angle of a cell DDALFA constant. Defining the radial size of a cell DR as constant we get a cell cross section area proportional to the radius R measured from the nozzle lip (point A).

The size of a cell: In order to get accurate simulated results it is recommended to define the size of a cell (DR and $R*DDALFA$) small compared with the mean free path of the molecules λ (typical $DR=\lambda/3$). However, as we do not expect to get large changes in flow parameters along the radius we may allow DR be much larger than $\lambda/3$. The angular size of the largest cell in a sector should comply with this requirement, but because of the computer limitation it is set to be equal to $5*\lambda$. This will be the basis for defining $DALFA$ for each sector.

C. INITIAL NUMBER OF MOLECULES IN CELLS

A "reasonable" number of molecules in a simulation is several thousands (a larger number, which is better, may be used for simple problems or when using a single user computer with large user memory space). The initial setting of molecules in cells is usually based on a guess of the number density in the specific cell. (The number of molecules in cells will change during the simulation according to the input/output calculated fluxes to the specific region).

The number density and the size of a cell are specified only in three dimensional flows. When applied to a two dimensional flow the simulation may be regarded as applying to an arbitrary thin slice of the real flow. In the axisymmetric flow we define the width of a cell by the angle DFI as shown in Figure (14), constant within a region.

The initial number density in cells of a given region is set constant. Defining the total number of simulated molecules in the region the number of molecules in each specific cell becomes a function of DFI . For example, assume that we limit the number of molecules in the smallest cell in the region to 15 then:

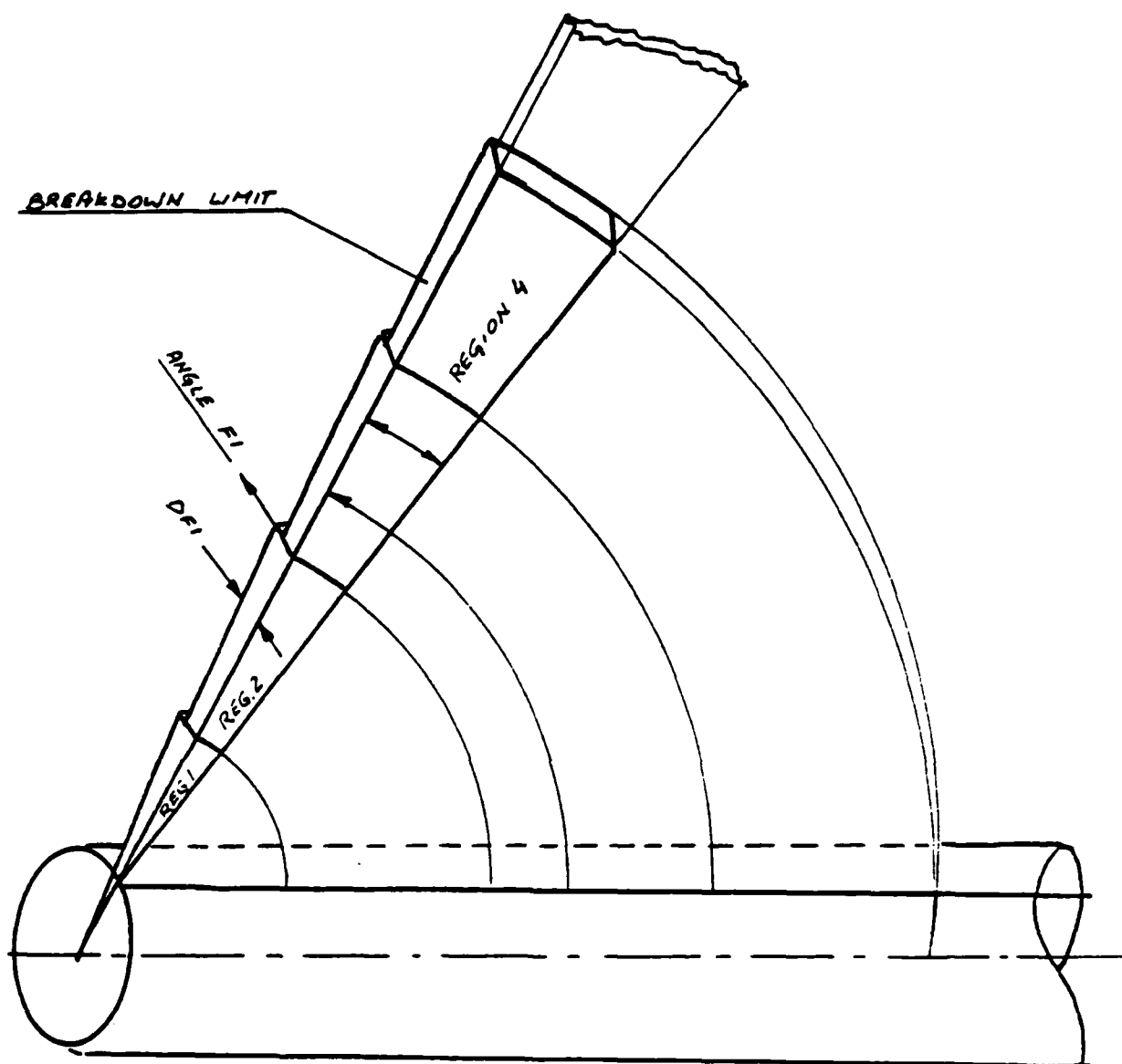


Figure 14. Variation of the angle DFI.

To maintain the number of simulated molecules within computational limits, the 'width' of each region defined by DFI is such that:

MIN = number of molecules in smallest cell in a region
 MIN = VOLUME (smallest cell) * number density
 = $f(R, ALFA, DALFA) * DFI * \text{number density for flux calculations}$

DFI is a weighting factor.

$$DFI*(contant) * (number\ density) = 15$$

Other cells contain the initial number of molecules proportional to their volumes.

D. DEFINITION OF INPUT AND OUTPUT FLOWS FOR A REGION

The cross sections of all regions (except those regions near the nozzle lips) are quadrilateral. Through the sides of the region molecules are allowed to enter or to leave according with the boundary conditions or as a result of molecular velocity. For the first sector, near the breakdown boundary the input flow (FWP1 and FWP2 see Figure (15)) is defined by the results from the continuum flow. FEN1, FNN1, FSN1, etc. are results of counting and averaging the outgoing molecules (the different vector names will be explained in Appendix B).

For the neighbor regions these output fluxes become inputs and have to be adjusted according to the differences in the angle DF1 of the different regions.

The simulation starts with regions in the sector near the breakdown boundary. At this time there is no data for input flows through faces E and N of the cell. An additional run of the whole program is required in order to take these calculated flows into account. If the accuracy of the results is important we may run this type of iteration several times until the results become stable. (Only after running the program for the whole domain once we shall be able to evaluate the importance of these iterations.)

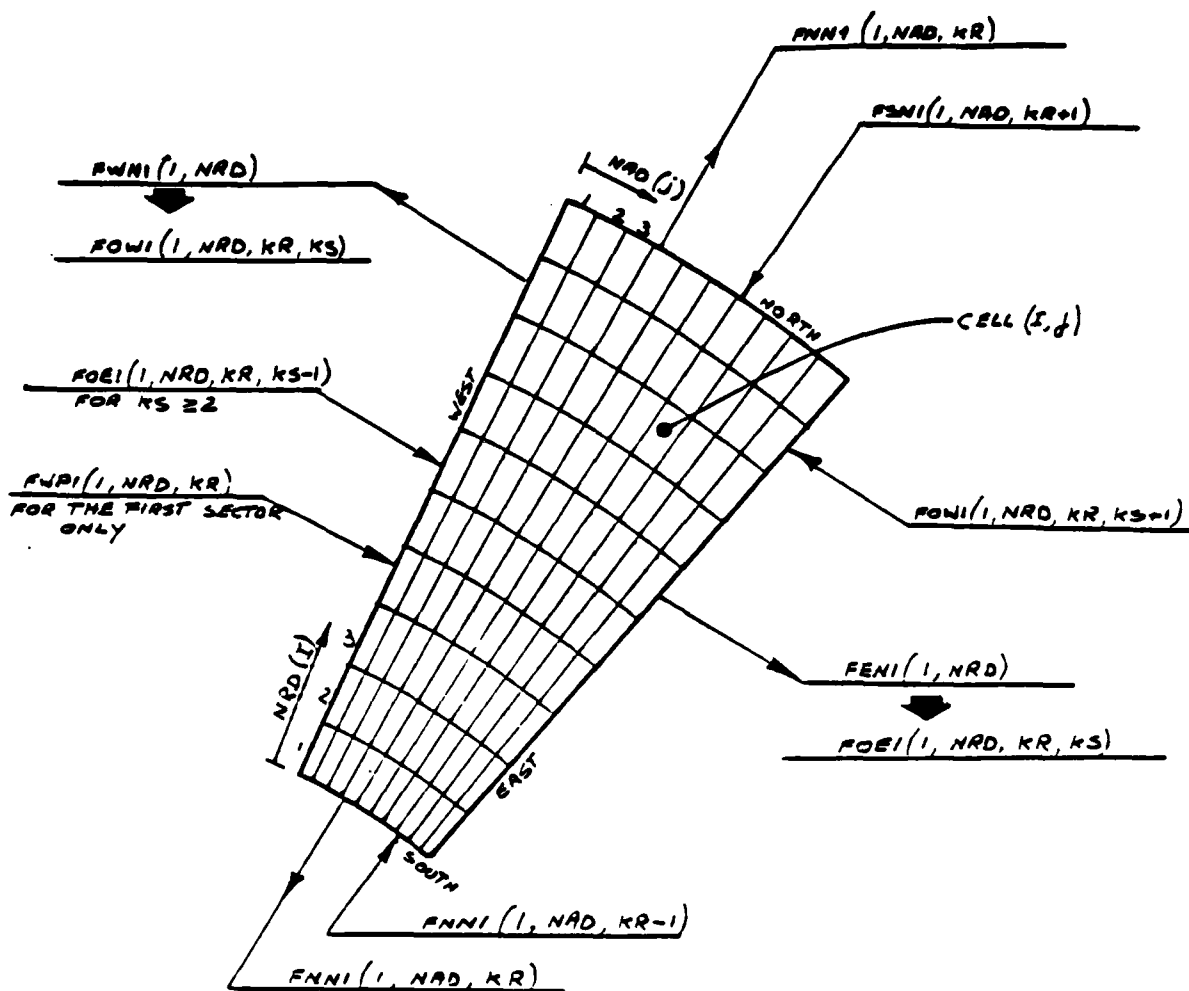


Figure 15. Definition of input and output flows of species 1 to a region (KR) in a sector (KS).

(For species 2 the flux names will change as follows:

instead $FWN1() \rightarrow FWN2()$

instead $FOW1() \rightarrow FOW2()$

etc.

E. COLLISIONLESS FLOW

In several sectors near the breakdown boundary we may find a high number density and the mean free path small compared with the size of a cell. There the calculated collisions are expected to have an influence on the flow parameters. For wider expansion angles the collisions become rare mainly because of the decrease in the density. In the ambient gas the mean free path (for 200 km altitude) is 240 m. Comparing this number with the size of the simulated domain may lead to the conclusion that there the flow may be regarded as collisionless.

We may define a limiting line in the flow where the collisions become insignificant. Consequently, molecules crossing this limit will in fact continue moving in straight lines; a part of them reach the solid wall.

Introducing this idea of the collisionless flow we may reduce the computation time and the memory requirements.

F. TWO DIMENSIONAL PLANAR FLOW VS. AXISYMMETRIC FLOW

The cell dimensions are completely specified only in three dimensional flow. When applied to two dimensional flow, the simulation may be regarded as applying to an arbitrarily thin slice of the real flow. The thickness of the slice may be chosen such that the number of simulated molecules complies with the cell volume and the physical number density. For the axisymmetric flow we have defined the angle DFI as the third coordinate so that the volume of the cell is completely specified.

Once the geometry is defined, the simulation may be accomplished and there is no difference if doing it for two dimensional or for axisymmetric flows.

APPENDIX A - THE AXSYM PROGRAM

A.1 DIFFERENT REGIONS IN THE JET

For the two dimensional jet with initial Mach number greater than unity the different regions are shown in Figure (16).

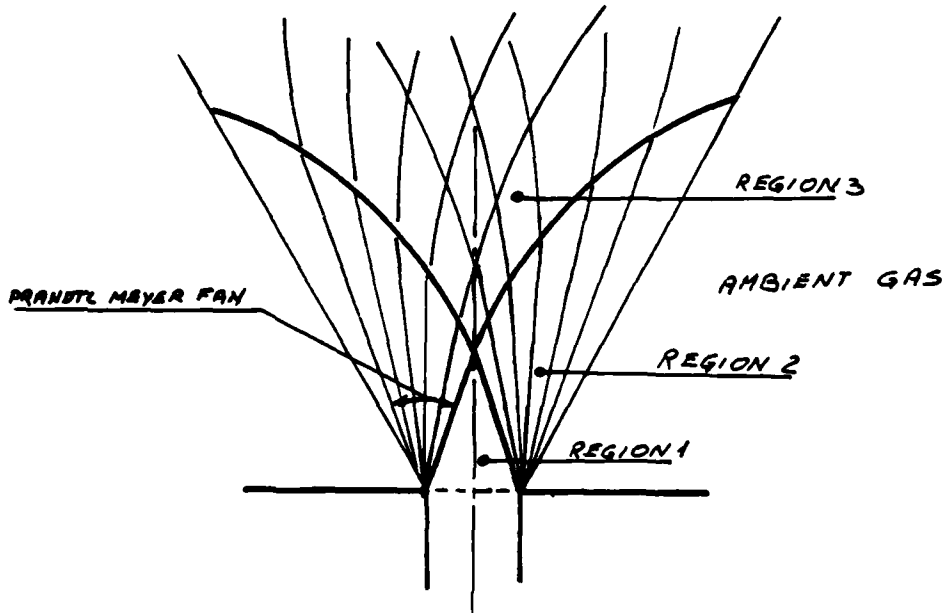


Figure 16. The three regions in an underexpanded jet.

For planar 2-D flow region 1 is a uniform flow core, region 2 is a simple region in which only one family of characteristics define the flow, and region 3 which contains the intersection of the two families of characteristics. Because our intention is to find solutions for highly underexpanded jets with very low ambient pressure, the calculation of further downstream flow is not necessary.

For the axisymmetric ring jet, we use the same definition for the different regions however, in this case none of the three regions has uniform flow and is not a simple region.

As shown in Equations (9,10) the PM function (v) and the flow direction (θ) of a point at location I,j may be calculated from the v and θ of two upstream points $(I-1,j)$ and $(I,j-1)$. Later, from the PM function at the new point we may derive the local Mach number, the local pressure, temperature, velocity and other thermodynamic parameters as required.

Definition of the mesh of points for the different regions is shown in Figure (17).

A.2 PROGRAM FLOWCHART

A simplified flowchart for the MOC program is shown in Figure (18). The program is designed to solve both axisymmetric as well as two dimensional flow

for $kD = 2$ it solves two dimensional flow

for $kD = 3$ it solves axisymmetric flow (This is also the default condition)

Initial data such as Mach number and pressure at the exit surface, ambient pressure and jet gas parameters are input data.

Output data contains the following for each mesh point:

Mach number, coordinates of mesh point (R,X), flow direction ($TETA$), pressure, temperature, local velocity, Knudsen number based on the distance between two points along a streamline, mean free path and breakdown parameter as defined by Bird.*

For each of the three regions, we start with precalculated boundary conditions enabling the calculation of the Mach angles, coordinates of mesh points and distances $d\xi$ and $d\eta$ as described in [2].

*For the exit plane instead the Bird's breakdown parameter, we calculate the ratio between time per three collisions and time of motion. Sometimes this ratio may be regarded as a measure of the breakdown of the continuum theory.

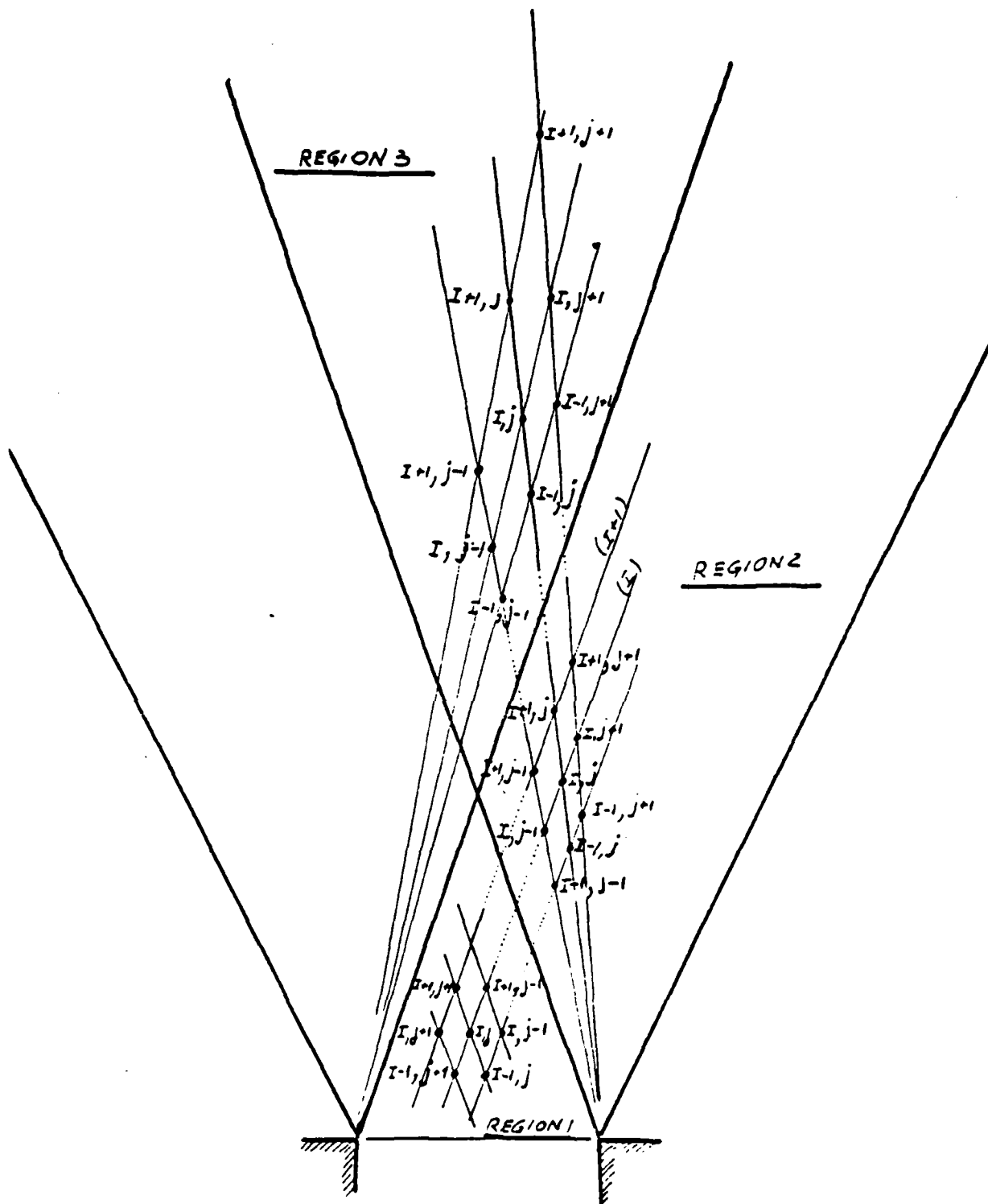


Figure 17. Indexing of mesh points for the different regions in the 'AXSYM' program.

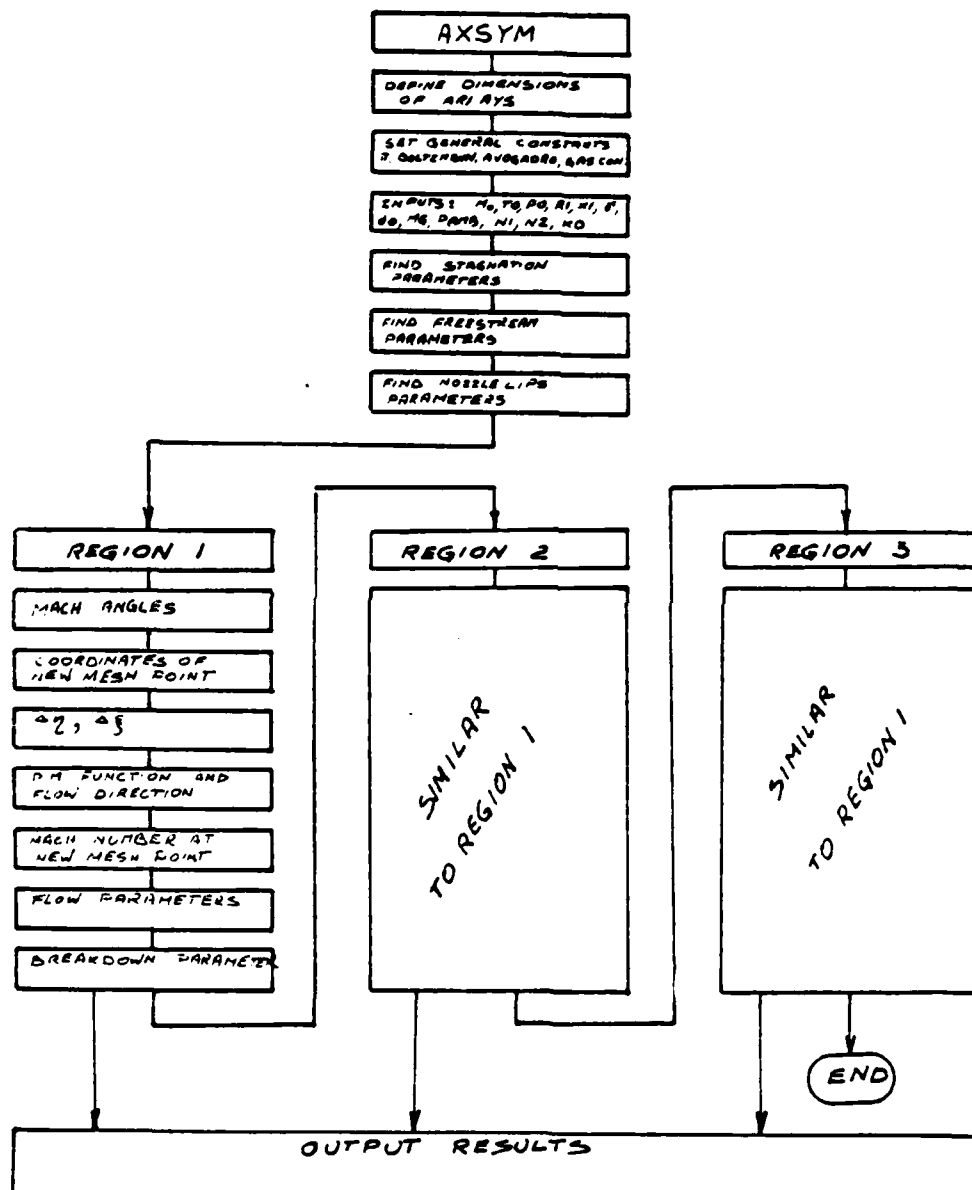


Figure 18. AXSYM Program Flowchart

The number of characteristics used in the program is arbitrary and depends on the required resolution (it may affect also the accuracy of the results and the amount of computation). We start with 20 characteristics along the exit cross section and with 50 characteristics in the Prandtl-Meyer fan thus a total of 70 characteristics of each family are calculated. In region 1 there are 20 left running and 20 right running characteristics. In region 2 there are 20 right running and 50 left running characteristics. In region 3 there are 50 left running and 50 right running characteristics.

In region 3 we limit the calculation where the two characteristics defining a new mesh point intersect at an angle smaller than the computational accuracy. In fact this occurs far downstream where continuum theory becomes invalid.

After defining the mesh geometry (successively) we calculate the Prandtl-Meyer function and flow direction, using equations (9,10).

The local Mach number is an implicit function of the Prandtl-Meyer angle. It is calculated by iterations with an initial guess of local Mach number set equal to a precalculated Mach number at an adjacent point, and the slope of the function as given by Equation (5). Figure (19) shows the iterative procedure for evaluating the Mach number at each mesh point.

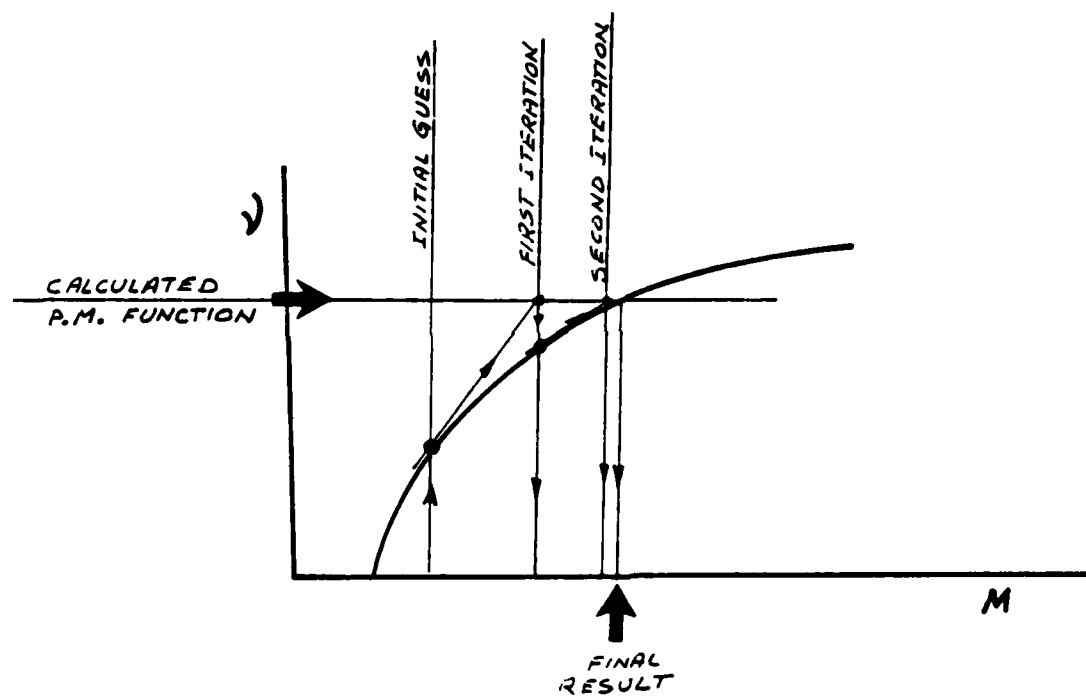


Figure 19. Iterative procedure for Mach number calculation.

Once the local Mach number has been found all other flow parameters may be defined using the Equation (1,2,3).

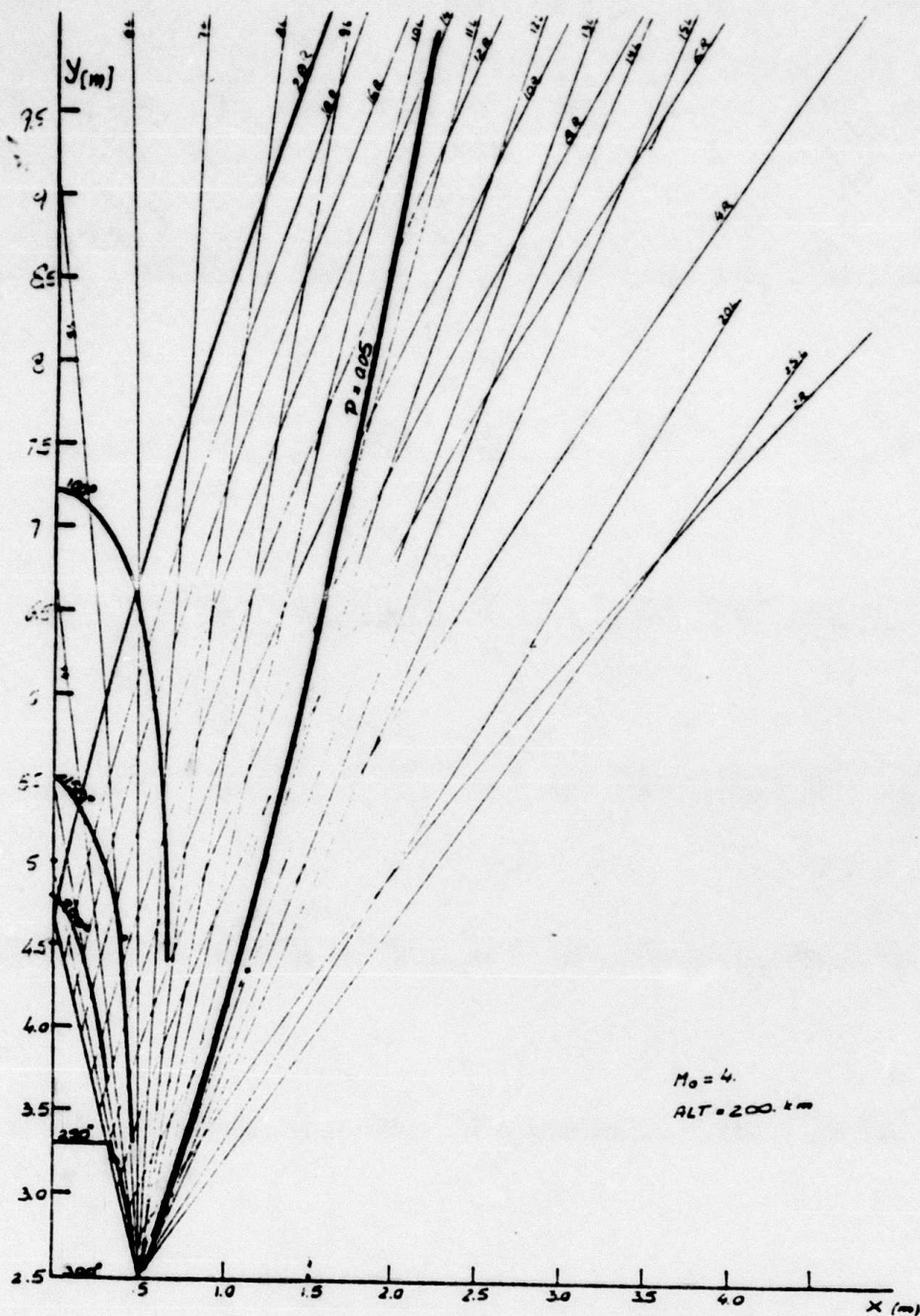


Figure 20. The mesh of characteristics in Region 2 and Region 3

Axisymmetric ring jet. $M_0 = 4$. Altitude=200km.

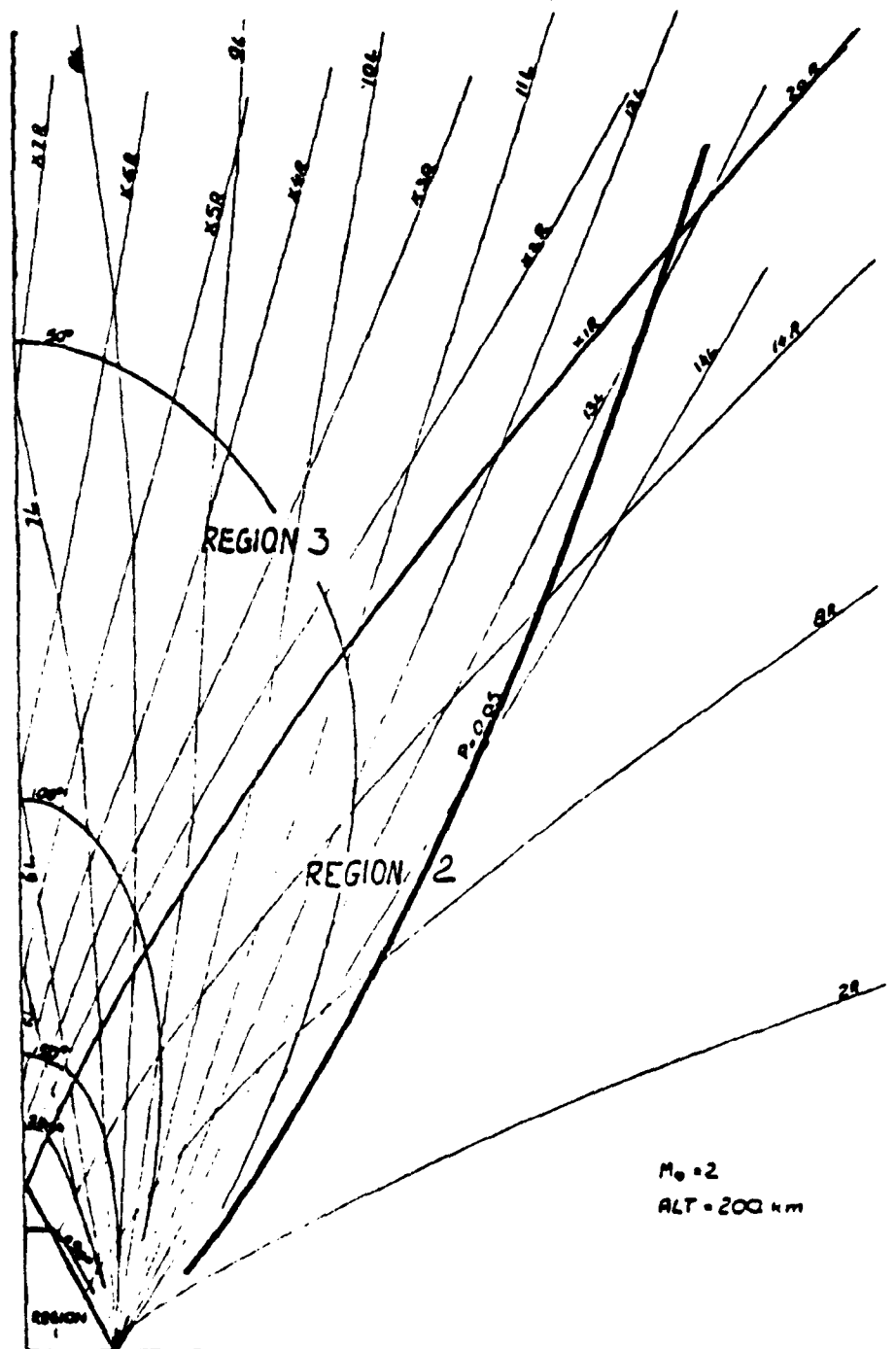


Figure 21. The mesh characteristics in Region 2 and Region 3
Axisymmetric ring jet. $M_0 = 2$. Altitude = 200km.

A.3 PROGRAM 'AXSYM' LISTING

```

$JOB
C PROGRAM AXSYM
C THIS PROGRAM CALCULATES THE ISENTROPIC EXPANSION OF A JET BY MEANS OF
C THE METHOD OF CHARACTERISTICS.
C FOR A TWO DIMENSIONAL JET 'KD' SHOULD BE SET EQUAL TO 2
C FOR AN AXISYMMETRIC RING JET 'KD' SHOULD BE SET EQUAL TO 3
C
C IMPLICIT REAL*8(A-H,O-Z,$)
C DIMENSION TETA(20,50),AM(20,50),R(20,50),X(20,50),PM(20,50)
C DIMENSION AMCOR(20,20),TETAC(20,20),XC(20,20),RC(20,20),PMC(20,20)
C DIMENSION DENSF(20,50)
C DIMENSION AMX(50,50),TETAX(50,50),XX(50,50),RX(50,50),PMX(50,50)
C
C TETA IS THE FLOW ANGLE (RADIAN) MEASURED FROM X AXIS.
C AM IS THE MACH NUMBER
C R IS THE RADIUS (NORMAL TO THE WALL)
C X IS THE AXIAL LOCATION (PARALLEL TO THE WALL)
C PM IS THE PRANDTL MEYER FUNCTION
C*****
C THE FOLLOWING IS DATA FOR THE SPECIFIC PROBLEM
C PAMB = 8.4736E-5
C KD = 3
C FOR TWO DIMENSIONAL FLOW KD=2 ,FOR AXISYMMETRICAL FLOW KD=3
C*****
C
C CONSTANTS
C PI = 3.141593
C BOLTZ = 1.38032E-23
C AVOG = 6.0225E+26
C RG = 8314.3
C
C EXIT SURFACE
C AMO = 4.00
C T0 = 300.0
C P0 = 136.0
C
C R1 = 2.5
C X1 = 0.5
C
C GAS DATA
C GAMA = 1.535
C DIAM = 2.95E-10
C GM = 17.0
C RJ = RG/GM
C CXS = PI*DIAM*DIAM
C GMM = GM/AVOG
C
C MESH DEFINITION
C N1=CHARACTERISTICS FROM THE EXIT PLANE
C N2=CHARACTERISTICS FROM THE CORNERS
C
C N1 = 20
C N2 = 50
C
C CONSTANTS FOR THE ISENTROPIC EXPANSION
C A1 = (GAMA-1.0)/GAMA
C B1 = 1.0/A1
C
C A2 = DSQRT((GAMA+1.)/(GAMA-1.))
C B2 = 1.0/A2
C
C A3 = (GAMA-1.)/2.
C
C C = MACH*MACH*A3 + 1.
C D = MACH*MACH -1.
C*****
C DEFINE STAGNATION PARAMETERS
C*****
C C = (1.0+A3*AMO*AMO)
C PRESSURE

```

```

AXS00010
AXS00020
AXS00030
AXS00040
AXS00050
AXS00060
AXS00070
AXS00080
AXS00090
AXS00100
AXS00110
AXS00120
AXS00130
AXS00140
AXS00150
AXS00160
AXS00170
AXS00180
AXS00190
AXS00200
AXS00210
AXS00220
AXS00230
AXS00240
AXS00250
AXS00260
AXS00270
AXS00280
AXS00290
AXS00300
AXS00310
AXS00320
AXS00330
AXS00340
AXS00350
AXS00360
AXS00370
AXS00380
AXS00390
AXS00400
AXS00410
AXS00420
AXS00430
AXS00440
AXS00450
AXS00460
AXS00470
AXS00480
AXS00490
AXS00500
AXS00510
AXS00520
AXS00530
AXS00540
AXS00550
AXS00560
AXS00570
AXS00580
AXS00590
AXS00600
AXS00610
AXS00620
AXS00630
AXS00640
AXS00650
AXS00660
AXS00670
AXS00680
AXS00690
AXS00700
AXS00710
AXS00720

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```

PN = C**B1
PSTG = P0*PN
C TEMPERATURE
TSTG = T0*C
C DENSITY
D0 = P0/(RJ*T0)
DSTG = PSTG/(RJ*TSTG)
C
C*****
WRITE(6,1)PSTG,TSTG,DSTG,DIAM,GM
1 FORMAT('0','STAGNATION PRESSURE=',E12.5,' TEMPERATURE=',F10.5,
1' DENSITY=',E12.5,' MOL.DIAM=',E12.5,' MOL.MASS=',F10.5)
WRITE(6,2)P0,T0,D0,AM0
2 FORMAT('0','EXIT PLANE PRESSURE=',E12.5,' TEMPERATURE=',F10.5,
1' DENSITY=',E12.5,' MACH=',F10.5)
C*****
C*****
C*****
C DEFINE FREE STREAM PARAMETERS AT THE RIGHT CORNER
C
C*****
C MACH NUMBER
FSM = DSQRT(((PSTG/PAMB)**A1-1.)/A3)
C TEMPERATURE
FST = TSTG/(1.+A3*FSM*FSM)
C DENSITY
FSD = PAMB/(RJ*FST)
C MACH ANGLES FOR HEAD AND TAIL OF FAN
AMIT = DARSIN(1./AM0)
AMIH = DARSIN(1./FSM)
C PRANDTL MEYER FUNCTION FOR HEAD AND TAIL OF FAN
D1 = DSQRT(AM0*AM0-1.)
D2 = DSQRT(FSM*FSM-1.)
PMH = A2*DATAN(B2*D2)-DATAN(D2)
PMT = A2*DATAN(B2*D1)-DATAN(D1)
C EXTERNAL TURNING ANGLE (FREE STREAM ANGLE)=EXTA
EXTA = PMH - PMT
C PRANDTL MEYER FAN ANGLE PMFA
PMFA = EXTA - AMIH + AMIT
C
C*****
C WRITE(6,3)PAMB,FST,FSD,FSM
3 FORMAT('0','FREE STREAM PRESSURE=',E12.5,' TEMPERATURE=',F10.5,
1' DENSITY=',E12.5,' MACH=',F10.5///)
C*****
C*****
C DEFINE THE MESH OF CHARACTERISTICS-AND FLOW PARAMETERS
C
C*****
C THE CORNER POINT - LEFT RUNNING CHAR.
C PMFA IS DEVIDED INTO N2 (=50) NONEQUAL DIVISIONS
C
RAT = (FSM/AM0-1)/0.02
RAT2 = FLOAT(N2-1)
E1 = DLOG(RAT)/DLOG(RAT2)
C
WRITE(6,4)
4 FORMAT('1','PRANDTL MEYER FAN LINE MACH
1 P.M. ANGLE TETA'//)
DO 20 N=2,N2
EN2 = FLOAT(N-2)
EN1 = FLOAT(N-1)
AMB = AM0*(1+.02*(EN2)**E1)
AMF = AM0*(1+.02*(EN1)**E1)
DELM = AMF-AMB
AM(1,N) = AMF
D1 = DSQRT(AM(1,N)*AM(1,N)-1.)
PM(1,N) = A2*DATAN(B2*D1)-DATAN(D1)
AMI = DARSIN(1./AM(1,N))
TETA(1,N) = PI/2.-(PM(1,N)-PMT)
C TETA IS THE FLOW ANGLE ON THE CHARACTERISTICS AT THE CORNER

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AXS01450
AXS01460
AXS01470
AXS01480
AXS01490
AXS01500
AXS01510
AXS01520
AXS01530
AXS01540
AXS01550
AXS01560
AXS0157
AXS01580
AXS01590
AXS01600
AXS01610
*AXS01620
AXS01630
*AXS01640
AXS01650
AXS01660
AXS01670
AXS01680
AXS01690
AXS01700
*AXS01710
*AXS01720
AXS01730
AXS01740
AXS01750
*AXS01760
AXS01770
AXS01780
AXS01790
AXS01800
AXS01810
AXS01820
AXS01830
AXS01840
AXS01850
AXS01860
AXS01870
AXS01880
AXS01890
AXS01900
AXS01910
AXS01920
AXS01930
AXS01940
AXS01950
AXS01960
AXS01970
AXS01980
AXS01990
AXS02000
AXS02010
AXS02020
AXS02030
AXS02040
AXS02050
AXS02060
AXS02070
AXS02080
AXS02090
PAXS02100
AXS02110
AXS02120
AXS02130
AXS02140
*AXS02150
*AXS02160

C		AXS02170
C	CALCULATE THE FLOW PARAMETERS IN THE CORE BOUNDED BY THE TWO MACH	AXS02180
C	WAVES STARTING AT THE NOZZLE LIPS (CORNER POINTS)	AXS02190
C	AT THE EXIT THE FLOW IS ASSUMED TO BE UNIFORM	AXS02200
C		AXS02210
C	*****	AXS02220
	WRITE (6,198)	AXS02230
198	FORMAT('1',' CORE '/')	AXS02240
	APM=0.	AXS02250
	BPM=0.	AXS02260
	CPM=0.	AXS02270
C		AXS02280
	DO 199 I = 2,N1	AXS02290
	WRITE (6,10)	AXS02300
	DO 199 J = 1,N1	AXS02310
	IF ((I+J-1).GT.N1) GO TO 199	AXS02320
	AMIL = DARSIN(1./AMCOR(I-1,J))	AXS02330
	ALFAL = PI-(TETAC(I-1,J)+AMIL)	AXS02340
C		AXS02350
	AMIR = DARSIN(1./AMCOR(I-1,J+1))	AXS02360
	ALFAR = TETAC(I-1,J+1)-AMIR	AXS02370
C		AXS02380
	XC(I,J) = (RC(I-1,J)-RC(I-1,J+1)+XC(I-1,J)*DTAN(ALFAL)+XC(I-1,J+1)*DTAN(ALFAR))/(DTAN(ALFAL)+DTAN(ALFAR))	AXS02390
	CENTR = DABS(XC(I,J))	AXS02400
	IF (CENTR.LT.0.001) XC(I,J) = 0.	AXS02410
	RC(I,J) = RC(I-1,J+1)+(XC(I,J)-XC(I-1,J+1))*DTAN(ALFAR)	AXS02420
C		AXS02430
	DKSI = DSQRT((XC(I,J)-XC(I-1,J+1))*2+(RC(I,J)-RC(I-1,J+1))*2)	AXS02440
	DETA = DSQRT((XC(I,J)-XC(I-1,J))*2+(RC(I,J)-RC(I-1,J))*2)	AXS02450
C		AXS02460
C		AXS02470
C	CALCULATE NOW THE PRANDTL MEYER FUNCTION AND FLOW ANGLE IN CORE.	AXS02480
	APM = PMC(I-1,J)+PMC(I-1,J+1)+TETAC(I-1,J+1)-TETAC(I-1,J)	AXS02490
	IF (KD.EQ.2) GO TO 151	AXS02500
	BPM = DSIN(AMIR)*DSIN(TETAC(I-1,J+1))/RC(I-1,J+1)*DKSI	AXS02510
	CPM = DSIN(AMIL)*DSIN(TETAC(I-1,J))/RC(I-1,J)*DETA	AXS02520
151	PMC(I,J) = (APM+BPM+CPM)/2.0	AXS02530
C		AXS02540
	APM = PMC(I-1,J+1)-PMC(I-1,J)+TETAC(I-1,J+1)+TETAC(I-1,J)	AXS02550
	TETAC(I,J) = (APM+BPM-CPM)/2.0	AXS02560
C		AXS02570
C	DEFINE MACH NUMBER (BY ITERATIONS)	AXS02580
C	INITIAL GUESS AMCOR(I,J)=AMCOR(I-1,J+1)	AXS02590
C		AXS02600
	AMG = AMCOR(I-1,J+1)	AXS02610
	KZ = 0	AXS02620
154	IF (KZ.GE.100) GO TO 160	AXS02630
	KZ = KZ+1	AXS02640
	C = AMG*AMG*A3+1.	AXS02650
	D = DSQRT(AMG*AMG-1.)	AXS02660
	PMCAL = A2*DATAN(B2*D)-DATAN(D)	AXS02670
	DELNI = PMCAL - PMC(I,J)	AXS02680
	DEL = DABS(DELNI)	AXS02690
	IF (DEL.LT..000002) GO TO 160	AXS02700
	IF (DELNI.LT.0.) GO TO 156	AXS02710
	AMG = AMG*.999	AXS02720
	GO TO 154	AXS02730
156	AMG = AMG*(1.-DELNI*C/D)	AXS02740
	GO TO 154	AXS02750
160	AMCOR(I,J) = AMG	AXS02760
C		AXS02770
C		AXS02780
C		AXS02790
C	CALCULATE FLOW PARAMETERS	AXS02800
	IF (J.GT.1) GO TO 197	AXS02810
	C = AMCOR(I,J)*AMCOR(I,J)*A3+1.	AXS02820
	PRES = PSTG/(C*B1)	AXS02830
	TEMP = TSTG/C	AXS02840
	DN = PRES/(BOLTZ*TEMP)	AXS02850
	FP = .707/(DN*CXS)	AXS02860
	SCALE = DKSI * DSIN(ALFAL)	AXS02870
	AKN = FP/SCALE	AXS02880

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SOUND = DSQRT(GAMA*RJ*TEMP)
VEL = SOUND*AMCOR(I,J)
C
C BREAKDOWN PARAMETER AS DEFINED BY 'BIRD'.
DENSF(I,J) = PRES/(RJ*TEMP)
DDENS = DENSF(I-1,J) - DENSF(I,J)
COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))
P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)
197 CONTINUE
C
C TIME1 = SCALE/VEL
C TIME2 = 3./((4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))))
C P = TIME2/TIME1
C*****AXS03020
C*****AXS03030
C*****AXS03040
WRITE(6,11)I,J,AMCOR(I,J),RC(I,J),XC(I,J),TETAC(I,J),TEMP,PRES,VELAXS03050
1,AKN,FP,DN,P
199 CONTINUE
C
C*****AXS03080
C*****AXS03090
C*****AXS03100
C MATCH CORE AND FAN POINTS
DO 200 I=1,N1
X(I,1) = XC(I,1)
R(I,1) = RC(I,1)
AM(I,1) = AMCOR(I,1)
PM(I,1) = PMC(I,1)
200 TETA(I,1) = TETAC(I,1)
C
C*****AXS03180
C*****AXS03190
C*****AXS03200
C CALCULATE FLOW PARAMETERS IN REGION 2 (SIMPLE PRANDTL MEYER FAN).
C
C*****AXS03240
WRITE(6,298)
298 FORMAT('1', ' REGION 2')
C
KFIN = 51
C
DO 299 I = 2,N1
WRITE(6,10)
DO 299 J = 2,N2
IF (J.GT.KFIN) GO TO 299
KZ = 0
AMIL = DARSIN(1./AM(I-1,J))
AMIR = DARSIN(1./AM(I,J-1))
ALFAL = PI-(TETA(I-1,J)+AMIL)
ALFAR = TETA(I,J-1)-AMIR
C
C CHECK ANGLES AND CALCULATE COORDINATES
ANGLE1 = PI/2.-.000001
ANGLE2 = PI/2+.000001
IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 201
X(I,J) = X(I-1,J)
GO TO 207
201 IF (ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 205
X(I,J) = X(I,J-1)
GO TO 207
C
205 X(I,J) = (R(I-1,J)-R(I,J-1)+X(I,J-1)*DTAN(ALFAR)+X(I-1,J)*DTAN(
1AL))/ (DTAN(ALFAL)+DTAN(ALFAR))
C
207 IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 209
R(I,J) = R(I-1,J)
GO TO 213
209 IF (ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 211
R(I,J) = R(I,J-1)
GO TO 213
C
211 R(I,J) = (X(I,J)-X(I,J-1))*DTAN(ALFAR)+R(I,J-1)

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213 DKSI = DSQRT((R(I,J)-R(I,J-1))**2+(X(I,J)-X(I,J-1))**2)
    DETA = DSQRT((R(I,J)-R(I-1,J))**2+(X(I,J)-X(I-1,J))**2)
C
    IF (R(I,J).GT.0..AND.X(I,J).GT.0.) GO TO 219
    KFIN = J-1
    WRITE(6,12)
12 FORMAT(' ',' FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')
219 CONTINUE
C LOCATION OF THE NEW MESH POINT HAS BEEN FOUND
C
C
C CALCULATE NOW PRANDTL MEYER FUNCTION AND FLOW DIRECTION FOR NEW POINT
    APM = PM(I,J-1)+PM(I-1,J)-TETA(I-1,J)+TETA(I,J-1)
    IF (KD.EQ.2) GO TO 251
    BPM = DSIN(AMIR)*DSIN(TETA(I,J-1))/R(I,J-1)*DKSI
    CPM = DSIN(AMIL)*DSIN(TETA(I-1,J))/R(I-1,J)*DETA
251 PM(I,J) = .5*(APM+BPM+CPM)
C
    APM = PM(I,J-1)-PM(I-1,J)+TETA(I,J-1)+TETA(I-1,J)
    TETA(I,J) = .5*(APM+BPM-CPM)
C
C CALCULATE NOW MACH NUMBER FOR EACH POINT
C INITIAL GUESS AM(I,J) = AM(I-1,J)
    AMG = AM(I-1,J)
    KZ = 0
254 IF (AMG.GT.200.) GO TO 257
    D = DSQRT(AMG*AMG-1.)
    GO TO 258
257 D = AMG
258 IF (KZ.GE.100) GO TO 260
    KZ = KZ + 1
    PMCAL = A2*DATAN(B2*D)-DATAN(D)
    DELNI = PMCAL - PM(I,J)
    DEL = DABS(DELNI)
    IF (DEL.LT..000002) GO TO 260
    IF (DELNI.LT.0.)GO TO 256
    AMG = AMG*.999
    GO TO 254
C//////////
256 IF (AMG.LT.2000.)GO TO 2560
    KFIN = J-1
    GO TO 299
C//////////
2560 D1 = (A3*AMG*AMG+1.)
    AMG = AMG*(1.-DELNI*D1/D)
    GO TO 254
C
260 AM(I,J) = AMG
C CALCULATE NOW LOCAL TEMPERATURE,PRESSURE,VELOCITY,KNUDSEN NO.
    C = AM(I,J)*AM(I,J)*A3+1
    PRES = PSTG/(C*B1)
    TEMP = TSTG/C
    DN = PRES/(BOLTZ*TEMP)
    DENSF(I,J) = PRES/(RJ*TEMP)
    DDENS = DENSF(I-1,J-1)-DENSF(I,J)
    SCALE = DSQRT((X(I,J)-X(I-1,J-1))**2+(R(I,J)-R(I-1,J-1))**2)
C*****
C
271 FP = .707/(DN*CXS)
C
    AKN = FP/SCALE
    SOUND = DSQRT(GAMA*RJ*TEMP)
    VEL = AM(I,J)*SOUND
C
C
    COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))
    P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)
C
C PRINT RESULTS FOR MESH POINTS
    KL = (-1)**I
    IF (KL.LT.0) GO TO 299
    WRITE(6,11)I,J,AM(I,J),R(I,J),X(I,J),TETA(I,J),TEMP,PRES,VEL,AKN,

```

1FP, DN, P	AXS04330
299 CONTINUE	AXS04340
C	AXS04350
C*****	AXS04360
C*****	AXS04370
C	AXS04380
C MATCH 'REGION 2' AND 'REGION 3' POINTS	AXS04390
C	AXS04400
C*****	AXS04410
L = KFIN- 1	AXS04420
DO 300 J = 1, L	AXS04430
XX(1, J) = X(20, J)	AXS04440
RX(1, J) = R(20, J)	AXS04450
AMX(1, J) = AM(20, J)	AXS04460
PMX(1, J) = PM(20, J)	AXS04470
300 TETAX(1, J) = TETA(20, J)	AXS04480
C*****	AXS04490
C*****	AXS04500
C	AXS04510
C CALCULATE FLOW PARAMETERS FOR REGION 3	AXS04520
C	AXS04530
C*****	AXS04540
WRITE (6, 397)	AXS04550
397 FORMAT ('1', ' REGION 3' /)	AXS04560
DO 399 I = 2, L	AXS04570
DO 399 J = I, L	AXS04580
IF (J.GT.KFIN) GO TO 399	AXS04590
IF (J.GT.I) GO TO 320	AXS04600
WRITE (6, 10)	AXS04610
320 KZ = 0	AXS04620
C	AXS04630
AMIL = DARSIN(1./AMX(I-1, J))	AXS04640
ALFAL = PI-(TETAX(I-1, J)+AMIL)	AXS04650
IF (J.GT.I) GO TO 301	AXS04660
ALFAR = ALFAL	AXS04670
TETAX(I, J) = PI*.5	AXS04680
TETAX(I, J-1) = PI-TETAX(I-1, J)	AXS04690
XX(I, J) = 0.	AXS04700
RX(I, J) = RX(I-1, J)+XX(I-1, J)*DTAN(ALFAL)	AXS04710
RX(I, J-1) = RX(I-1, J)	AXS04720
XX(I, J-1) = -XX(I-1, J)	AXS04730
DKSI = (RX(I, J)-RX(I-1, J))/DSIN(ALFAL)	AXS04740
DETA = DKSI	AXS04750
PMX(I, J-1) = PMX(I-1, J)	AXS04760
GO TO 316	AXS04770
301 AMIR = DARSIN(1./AMX(I, J-1))	AXS04780
ALFAR = TETAX(I, J-1)-AMIR	AXS04790
C	AXS04800
IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 302	AXS04810
XX(I, J) = XX(I-1, J)	AXS04820
GO TO 307	AXS04830
302 IF (ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 305	AXS04840
XX(I, J) = XX(I, J-1)	AXS04850
GO TO 307	AXS04860
305 XX(I, J) = (RX(I-1, J)-RX(I, J-1)+XX(I, J-1)*DTAN(ALFAR)+XX(I-1, J)*DTA	AXS04870
1N(ALFAL))/(DTAN(ALFAL)+DTAN(ALFAR))	AXS04880
C	AXS04890
307 IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 309	AXS04900
RX(I, J) = RX(I-1, J)	AXS04910
GO TO 315	AXS04920
309 IF (ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 311	AXS04930
RX(I, J) = RX(I, J-1)	AXS04940
GO TO 315	AXS04950
311 RX(I, J) = RX(I, J-1)+(XX(I, J)-XX(I, J-1))*DTAN(ALFAR)	AXS04960
C	AXS04970
315 DKSI = DSQRT((RX(I, J)-RX(I, J-1))*2+(XX(I, J)-XX(I, J-1))*2)	AXS04980
DETA = DSQRT((RX(I, J)-RX(I-1, J))*2+(XX(I, J)-XX(I-1, J))*2)	AXS04990
316 CONTINUE	AXS05000
C	AXS05010
IF (RX(I, J).GE.0..AND.XX(I, J).GE.0.) GO TO 319	AXS05020
KFIN = J-1	AXS05030
WRITE (6, 398)	AXS05040

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398 FORMAT (' ','FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')AXS05050
C AXS05060
C LOCATION OF THE NEW POINT HAS BEEN FOUND AXS05070
C*****AXS05080
C AXS05090
C CALCULATE NOW P.M. ANGLE AND FLOW DIRECTION AXS05100
319 APM = PMX(I,J-1)+PMX(I-1,J)-TETAX(I-1,J)+TETAX(I,J-1) AXS05110
    IF(KD.EQ.2) GO TO 351 AXS05120
    BPM = DSIN(AMIR)*DSIN(TETAX(I,J-1))/RX(I,J-1)*DKSI AXS05130
    CPM = DSIN(AMIL)*DSIN(TETAX(I-1,J))/RX(I-1,J)*DETA AXS05140
351 PMX(I,J) = .5*(APM+BPM+CPM) AXS05150
    APM = PMX(I,J-1)-PMX(I-1,J)+TETAX(I,J-1)+TETAX(I-1,J) AXS05160
    TETAX(I,J) = .5*(APM+BPM+CPM) AXS05170
C AXS05180
C CALCULATE NOW THE MACH NUMBER FOR EACH POINT AXS05190
C INITIAL GUESS AMX(I,J) = AMX(I-1,J) AXS05200
    AMG = AMX(I-1,J) AXS05210
    KZ = 0 AXS05220
    KH=0 AXS05230
    KL=0 AXS05240
354 IF (AMG.GT.2000.) GO TO 357 AXS05250
    D = DSQRT(AMG*AMG-1.) AXS05260
    GO TO 358 AXS05270
357 D = AMG AXS05280
358 IF (KZ.GE.50)GO TO 360 AXS05290
    KZ = KZ +1 AXS05300
    PMCAL = A2*DATAN(B2*D)-DATAN(D) AXS05310
    DELNI = PMCAL-PMX(I,J) AXS05320
    DEL = DABS(DELNI) AXS05330
    IF (DEL.LT..000002) GO TO 360 AXS05340
    IF (DELNI.LT.0.)GO TO 356 AXS05350
    AMG = AMG*.98 AXS05360
    GO TO 354 AXS05370
356 IF (AMG.LT.5000.) GO TO 3560 AXS05380
    KFIN = J-1 AXS05390
    GO TO 399 AXS05400
3560 D1 = A3*AMG*AMG+1. AXS05410
C*****AXS05420
    DDELNI = DELNI AXS05430
    IF (AMG.GT.20.) DDELNI = DELNI*(.95**KZ) AXS05440
C*****AXS05450
    AMG = AMG*(1.-DDELNI*D1/D) AXS05460
    GO TO 354 AXS05470
360 AMX(I,J) = AMG AXS05480
C AXS05490
C CALCULATE NOW THE LOCAL TEMPERATURE, PRESSURE, VELOCITY, KNUDSEN AXS05500
    C = AMX(I,J)*AMX(I,J)*A3+1. AXS05510
    PRES = PSTG/(C**B1) AXS05520
    TEMP = TSTG/C AXS05530
    DN = PRES/(BOLTZ*TEMP) AXS05540
C*****AXS05550
    DENSF(I,J)=PRES/(RJ*TEMP) AXS05560
    DDENS=DENSF(I-1,J-1)-DENSF(I,J) AXS05570
    FP = .707/(DN*CXS) AXS05580
    SCALE=DSQRT((XX(I,J)-XX(I-1,J-1))*2+(RX(I,J)-RX(I-1,J-1))*2) AXS05590
    AKN=FP/SCALE AXS05600
C AXS05610
C AXS05620
C*****AXS05630
C ALFALL = -ALFAL+PI AXS05640
C AF = ALFALL-PI/2. AXS05650
C AF = DABS(AF) AXS05660
C IF (AF.LT..000001) GO TO 370 AXS05670
C BF = 1./DSQRT(1. + DTAN(ALFALL)**2) AXS05680
C SCALE=BF*(RX(I,J-1)-DTAN(ALFALL)*(XX(I,J-1)-XX(I-1,J))-RX(I-1,J)) AXS05690
C SCALE = DABS(SCALE) AXS05700
C*****AXS05710
    SOUND = DSQRT(GAMA*RJ*TEMP) AXS05720
    VEL = AMX(I,J)*SOUND AXS05730
C AXS05740
    COLF=4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM)) AXS05750
    P=VEL*DDENS/(SCALE*DENSF(I,J)*COLF) AXS05760

```

C		AXS05770
C	PRINT RESULTS	AXS05780
	WRITE(6, 11)I,J,AMX(I,J),RX(I,J),XX(I,J),TETAX(I,J),TEMP,PRES,VEL,	AXS05790
	1AKN,FP,DN,P	AXS05800
399	CONTINUE	AXS05810
	STOP	AXS05820
	END	AXS05830
\$ENTRY		AXS05840

A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM'.

Parameter Name	Physical Name	Units	Type	Description
PAMB	ambient pressure	pascals	real	ambient atmosphere pressure
KD	K dimensions	-	integer	KD=2 for two dimensional jet KD=3 for axisymmetric ring jet
PI	π	-	real constant	
BOLTZ	Boltzmann constant	$\frac{\text{Joule}}{\text{degree}}$	real	1.38032×10^{-23} joules/degree
AVOG	Avogadro's constant	$\frac{\text{molecules}}{\text{mol}}$	real	6.0225×10^{26} 1/kmol
RG	Universal gas constant	$\frac{\text{Joule}}{\text{mol.deg}}$	real	8314.3
AM0	Mach No. (E.P)	-	real	Mach number at exit plane
T0	Temperature (E.P)	$^{\circ}\text{k}$	real	Temperature at exist plane
P0	Pressure (E.P)	pascals	real	Pressure at exit plane
R1	Cylinder radius	m	real	Radius of the cylindrical vehicle
X1	0.5* nozzle width	m	real	Half width of nozzle
GAMA		-	real	averaged heat capacity ratio (jet)
DIAM	Molecule diameter	m	real	averaged molecular diameter (jet)
GM	Molecular mass	kg/kmol	real	averaged molecular weight (jet)
RJ	Gas constant	$\frac{\text{joules}}{\text{kJ.deg}}$	real	gas constant (jet)
CXS		m^2	real	collision cross section (hard sphere)
GMM	mass of a molecule	kg	real	averaged mass of a molecule
N1			integer	number of divisions (characteristics from the exist plane)
N2			integer	number of characteristics in the Prandtl Meyer fan
A1			real	$\frac{\gamma - 1}{\gamma}$
B1			real	$\frac{\gamma}{\gamma - 1}$

A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

Parameter Name	Physical Name	Units	Type	Description
A2			real	$[(\gamma + 1)/(\gamma - 1)]$
B2			real	$1/A2$
A3			real	$\frac{\gamma - 1}{2}$
C			real	$M^2 \frac{\gamma - 1}{2} + 1$
D, D1, D2			real	$M^2 - 1$
PSTG		pascals	real	stagnation pressure
TSTG		$^{\circ}k$	real	stagnation temperature
DSTG		kg/m^3	real	stagnation density
FSM			real	free stream Mach number
FST		$^{\circ}k$	real	free stream temperature
FSD		kg/m^3	real	free stream density
AMIT	μ_T	radius	real	Mach angle (tail of P.M. fan)
AMIH	μ_H	radius	real	Mach angle (head of P.M. fan)
PMT	ν_T	radius	real	P.M. function (tail)
PMH	ν_H	radius	real	P.M. function (head)
RAT, RAT2, E1			real	used to define a logarithmic division of the corner characteristics (50 lines in P.M. fan)(a linear division would have resulted in concentration of characteristics at high Mach numbers)
DELM			real	difference of Mach numbers
AM(I,J)	M		real 2-D array	Mach number at location (I,j)(used for the corner)
PM(I,J)	ν	radius		P.M. function at location (I,j)(used for the corner)
AMI	μ	radius	real	Mach angle
R(I,J)		m	real 2-D array	radius (or ordinate) at (I,j)
TETA(I,J)	θ	radius	real 2-D array	flow direction at (I,j)

A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

Parameter Name	Physical Name	Units	Type	Description
ALFAL		radians	real	angle of a left running characteristics
ALFAR		radians	real	angle of a right running characteristics
DENSF(I,J)		kg/m ³	real 2-D array	gas density at point LJ
AMCOR(I,J)			real 2-D array	Mach number at mesh points in region (1) (region 1 is bounded by the two tail characteristics)
TETAC(I,J)		radians	real 2-D array	flow direction at mesh points (region 1)
PMC(I,J)		radians	real 2-D array	P.M. function at mesh points (region 1)
XC(I,J)		m	real 2-D array	X coordinate at mesh points (region 1)
RC(I,J)		m	real 2-D array	radius (ordinate) at mesh points (region 1)
AMIL		radians	real	Mach angle far left running characteristics
AMIR		radians	real	Mach angle far right running characteristics
DKSI	dξ	m	real	distance between mesh points
DETA	dη	m	real	distance between mesh points
DELNI	dv	radians	real	P.M. differential
AMG		radians		Mach number (used for iterative calculation)
PRES				pressure
TEMP				temperature
DN				number density
FP				mean free path
AKN				Knudsen number
SOUND				speed of sound
VEL				absolute local velocity
DDENS				density difference between two points along a streamline
COLF				collision frequency
P				breakdown parameter

A.5 AXSYM PROGRAM USER'S GUIDE

1. Input data:

ambient pressure	PAMB
Mach number (Exit plane)	AMO
Temperature (Exit plane)	TO
Pressure (Exit plane)	PO
Half width of nozzle	X1
Radius of nozzle ring	R1
Specific heat ratio of jet gas	GAMMA
average molecular diameter (jet)	DIAM
average molecular weight	GM

2. Options for flow geometry

two dimensional flow	KD=2
ring jet	KD=3
default condition	KD=3

3. Resolution of mesh points

to change the resolution of the mesh points

a - change N1 and N2 as necessary

b - change 'DIMENSIONS' according to new values of N₁ and N₂

c - define distribution of Mach lines in the Prandtl-Meyer fan as required

(program lines 126-131)

4. Execution commands:

After copying program into USER'S FILE:

```
WATFIV AXSYM * (XTYPE
```

The program will run on user's terminal under WATFIV. A soft copy of program listing and output listing will be stored in user's disk named AXSYM LISTING.

5. Hard Copy

PRINT AXSYM LISTING.

6. Program Outputs.

All necessary outputs are automatically listed by the program.

Figure (20) and Figure (21) show the resulting mesh of characteristics calculated for an altitude of 200 km for $M_0=4$ and $M_0=2$ respectively.

In these figures we also show some isotherms and the limit where the breakdown parameter equals 0.05. These lines are plotted (manually) using interpolation procedures. Data along the breakdown line is input data for the molecular flow.

APPENDIX B SIMUL PROGRAM

B.1 DATA ORGANIZATION

Because of the large number of molecules, cells, regions and sectors in the simulation and the large number of data related to each molecule, each cell and region to be stored, special precautions should be taken in order not to overflow the available computer memory.

The following data organization was used in SIMUL. Figure 22 shows the geometry of one sector.

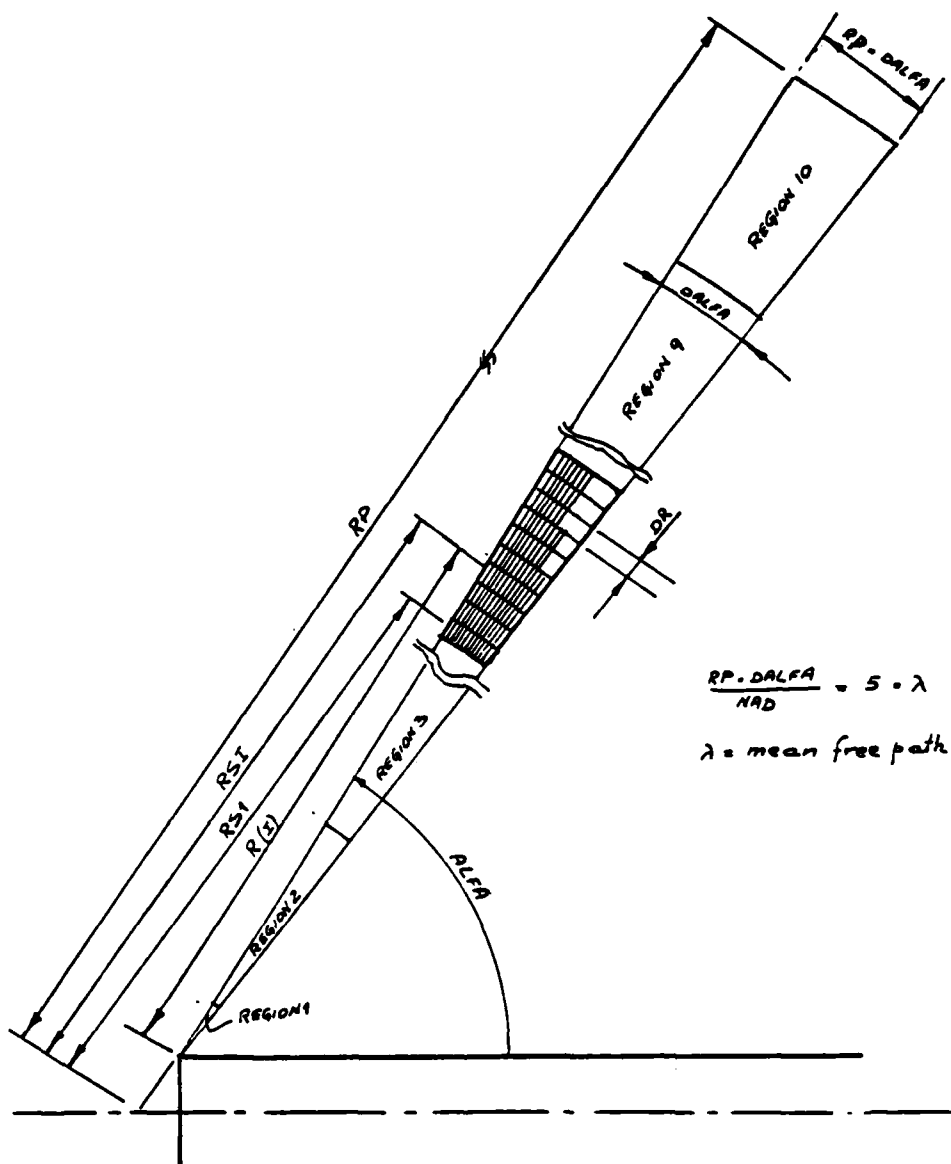


Figure 22. Definition of sector geometry and cell volume.

cell volume = $v(I) = R(I) * DDALFA * DR * RSI * DFI$.

$$\frac{v(I)}{v(1)} = \frac{R(I) \cdot RSI(I)}{R(1) \cdot RSI}$$

$v(1)$ is the volume of smallest cell in a region.

1. Tables of Molecules and Their Parameters

P1(L,N1M) - Light molecules of the jet

P2(L,N2M) - Heavy molecules of the jet

P3(L,N3M) - Ambient gas molecules (not used in the present program)

N1M, N2M, N3M - maximum number of molecules in simulation. Number of active molecules may be smaller or equal to (N<I>M).

L=1,2,3 - cartesian components of velocity v_x, v_y, v_z [m/s]

L=4 - radial coordinate [meters]

if $r=-99$ the particular molecule is inactive

L=5 - angular coordinate [radians].

This table is generated each time the simulation is initiated for a region.

That means, the same group of molecules (as stored in the computer memory) is used to simulate the flow in all regions in the computation domain.

2. C(M,I,j) Table of Cells (in a Region)-Real Data

- I = 1,10 - radial index of the cell in a region
- j = 1,10 - angular index of the cell in a region
- M = 19 - radial coordinate of cell center
- M = 20 - angular coordinate of cell center
- M = 1,9 - time parameter for collisions of different species in a
cell
- M = 10-18 - maximum relative velocity expected for collisions of
different species in a cell

3. IP(N1A+N2A+N3A) Table of the addresses of the active molecules
arranged in order of their species and in the order of their cells

IC(N,I,j) - table of cells (in a region) integer data

I = 1,10 - radial index

j = 1,10 - angular index

N = 1 - number of molecules (spec 1)

N = 2 - number of molecules (spec 2)

N = 3 - number of molecules (spec 3)

N = 4 - (starting address - 1) of molecules as ordered in (IP).

4. Reg(N,kR,kS) Data table for a specific region (real)

kR = 1,10 - index of a region in a sector

kS = 1,20 - index of the sector

N = 1 - Df1 = differential angle (axisymmetric)

Df1 is a weighting factor

N = 2 - DN1 = number density (species 1)

N = 3 - DN2 = number density (species 1)

N = 4 - VOL 1 = actual volume of smallest cell in kR

N = 5 - AREA1 INPUT area of smallest cell in kR

5. Region Geometry and Input Flux

R(10) - polar radius of a cell in a region

A(10) - $\frac{\text{input area of a cell}}{\text{input area of smallest cell}}$

VOL(10) - $\frac{\text{volume of a cell}}{\text{volume of smallest cell}}$

M1(10) - initial number of molecules in cells
(equal number of molecules of either jet species)

F1(10), F2(10) - input flux through high pressure starting line
(spec 1), (spec 2)

6. Input Flux From High Pressure Starting Line

FWP1(N,I,j)

FWP2(N,I,j)

```

↑↑↑↑
| species
| positive (input molecules)
| west
| flux

```

I = 1,10 - number of the cell along the starting line in a region
(j)

j = 1,10 - number of the region along the starting line

N = 1 - molecular flow for a given DF1

N = 2 - mean molecular velocity Vx

N = 3 - mean molecular velocity Vy

N = 4 - mean input gas temperature

7. Output Flux

FNN1(4,NAD,kR)

FSN1(4,NAD,kR)

FNN2(4,NAD,kR)

FSN2(4,NAD,kR)

```

↑↑      ↑↑
| negative (output)  | negative (output)
| north              | south

```

kR - number of region in the sector

NAD - angular location

The first index include the same parameters as (FWP1)

FEN1(4,NRD)

FWN1(4,NRD)

FEN2(4,NRD)

FWN2(4,NRD)

```

↑↑      ↑↑
| negative      | negative
| east          | west

```

NRD → radial location

FEN1, FEN2, FWN1, FWN2 are necessary for iterations within one sector.

8. Sampling of Output Flux from a Sector

After averaging they are transferred to FOE1, FOE2, FOW1, FOW2.

FOW1(4, kC, kR, kS)

output flow to the west

FOW2(4, kC, kR, kS)

FOE1(4, kC, kR, kS)

output flow to the east

FOE2(4, kC, kR, kS)

kC - radial location (cell) of flow in a region

kR - index of a region in a sector

kS - index of the sector

The first index (4 parameters) include the same parameters as FEPl().

B.2 MOLECULAR SIMULATION FOR A GIVEN REGION

After we define the geometry of the whole sector resulting from the region geometry and cell geometry, we may start with the molecular simulation.

This includes:

- initial setting of molecules in cells
- molecules are moved according to the time increment Δt
- new molecules are generated according to input (or output) flows
- collisions calculations
- integration of flow parameters for average parameters calculations
- repetition of the whole procedure as long as necessary to obtain reasonable statistical averaging
- calculate averages and flow weighting.

These routines are the core of the program and must be repeated for all regions in a sector and (or all sectors in the domain where the collisions are significant).

In the following sections we bring a detailed description of this part of the program.

1. Initial Setting of Molecules in Cells

- a. The initial number of available molecules in a simulation is larger than the number of active molecules ($P1(\text{data}, \text{number of molecules})$, $P2(\text{data}, \text{number of molecules})$ are the vectors used for species 1 and 2)
- b. an inactive molecule is defined as

$$[P1(4,N) \text{ or } P2(4,N)] = -99$$

- c. calculation of number of molecules to be set in each cell
- d. calculation of cell coordinates
- e. deactivation of all available molecules in simulation
- f. definition of molecules coordinates

P1(4,N), P2(4,M) are polar radiuses

P1(5,N), P2(5,M) are angular coordinate in radians

All molecules in a cell are set at random locations within the cell.

- g. definition of molecular velocities

P1(1,N), P2(1,M) velocity in X direction

P1(2,N), P2(2,M) velocity in Y direction

P1(3,N), P2(3,M) velocity in Z direction

Thermal velocities are random function of temperatures and are added to the mean velocity as defined at initial boundary $ALFA_0$ of the region.

As the thermal velocity has a Boltzmann distribution the thermal velocity setting is based on rejection-acceptance methods (for more details see Bird [4] Appendix D).

- h. reset collision timers and relative velocity

1. reset general time counter: Time = 0

3. The Simulation

- a. Move all molecules according to their velocity (V_x , V_y) and find their new coordinates

Note - A routine designed to calculate the collisions with the wall was included in the program; if the region (or sector) is bounded by the solid wall, the collision is calculated - resulting new velocities and directions and counted for wall flux calculations. If the program is stopped at an angle where the flow becomes collisionless, this routine becomes irrelevant and other type of calculations should be designed.

- b. Output flow counting: all molecules that leave the region are counted and stored in specific vectors which are used as inputs to other regions. The output vectors are (X represent 1 or 2 for the two species in the program (FSNX))

FSNX(1,j,kR) → "south" boundary

FNNX(1,j,kR) → "north" boundary

FENX(1,I) → "east" boundary

FWNX(1,I) → "west" boundary

I represents the radial location index of the cell

j represents the angular location index

kR is the index of the region within a sector

Note - all molecules that move to

(j=NAD+1)(I=NRD+1) are placed in FENX(1,NRD)

(j= -1)(X=NRD+1) are placed in FWNX(1,NRD)

(j=NAD+1)(I= -1) are placed in FSNX(1,1,kR)

(j= -1)(I= -1) are placed in FWNX(1,1,kR)

This was done only for simplification reasons.

- c. Generation of new molecules due to input flows. Through the four sides E,N,W,S, of a region, molecules are allowed to enter the region according with the flows coming from the neighbouring regions:

for "W" side of the region in sector 1

FWPX(P,I,kR)

for other sectors

FOEX(P,I,kR,kS-1)

for "E" side of any region

FOWX(P,I,kR,kS+1)

for "N" side of any region

FSNX(P,j,kR+1)

for "S" side of the region

FNNX(P,j,kR-1)

The first parameter of all these arrays represent:

P = 1 - number flux (real number)

P = 2 - velocity component - (V_x)

P = 3 - velocity component - (V_y)

P = 4 - gas temperature

Note 1 - because every region has a different size of angle DFI, all fluxes have to be adjusted accordingly.

Note 2 - input fluxes are calculated, adjusted and stored as real numbers. The number of input molecules are by definition integers. In order not to "lose" molecules, the number of input molecules is increased by 1 on a random basis. (The average of many runs will result in the accurate average input flow.)

New molecules are set at random locations on the boundary of the specific cells and at random time within DTM. Then each molecule is allowed to enter the region according to its initial coordinate and velocity. At the end of the time interval the new location and velocity is stored in molecule array P1 or P2. If DTM is chosen to be too large and cell size is small (total region size too small) some molecules may cross the region and will not be counted in the simulation of the specific region. In order not to "lose" molecules:

- (a) DTM should be decreased
- (b) count these molecules as output fluxes from the specific region. (This is recommended only if there is no other choice.)

Note - Because the arrays of input flows store only averaged data for the molecules, the thermal velocity of each new molecule is calculated according to the Boltzmann distribution as a function of the averaged temperature.

- d. Rearrangement of molecules in cells. Before collisions are calculated all simulated molecules which have been let to move and generated have to be rearranged and recounted for each cell.

The array $IC(k,I,j)$ contains integer data for each cell
 (I,j)

$k = 1$ - is the number of molecules of species 1

$k = 2$ - is the number of molecules of species 2

$k = 3$ - is the number of molecules of species 3 (not used)

$k = 4$ - is the (address-1) of the first molecule in the cell

related to the vector $IP(M)$

Vector $IP(M)$ contains the list of the simulated molecules arranged
in the order of species in cells and cells respectively. The
following is a graphic description of $IP(M)$

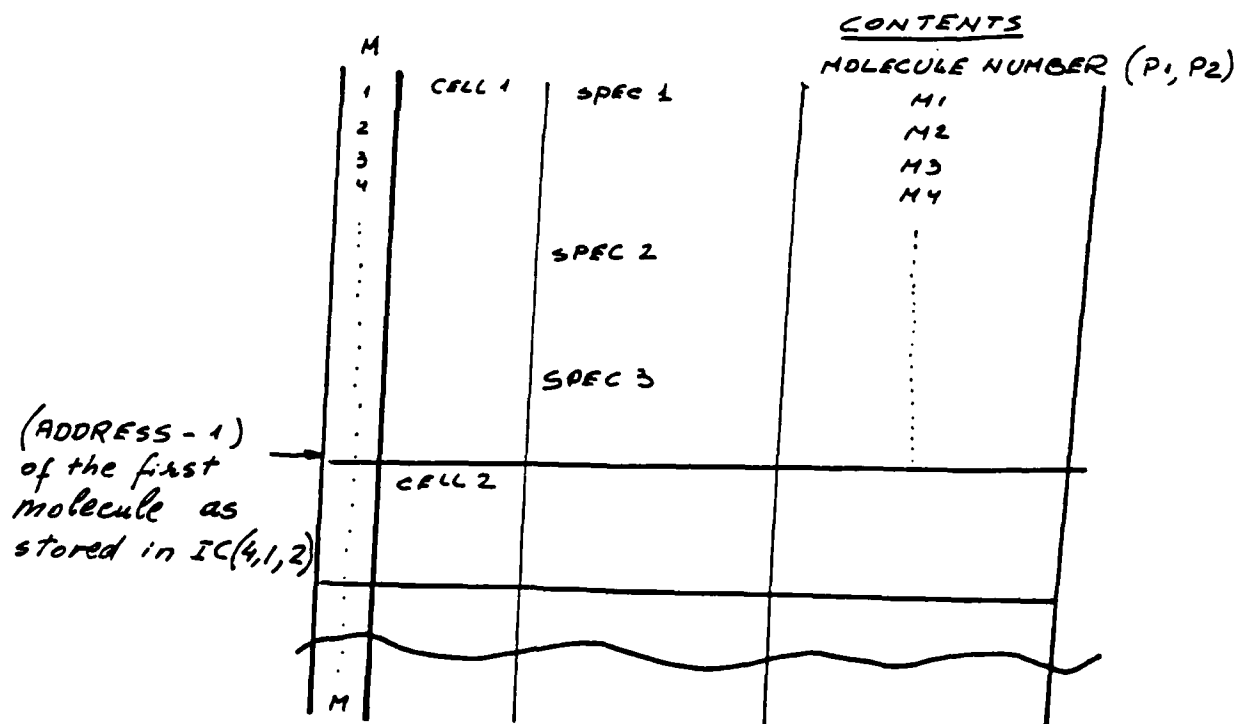


Figure 23. Vector $IP(M)$

B.3 SIMUL Program Flowchart

A simplified flowchart for the Monte Carlo simulation of the molecular flow is shown in Figure 24. The program is designed to solve the ring axisymmetric jet flow, however, minor changes may be done to enable a different geometry.

B.4 SIMUL Program Listing

```

C      PROGRAM SIMUL
C THIS PROGRAM IS DESIGNED TO CALCULATE THE MOLECULAR FLOW OUTSIDE THE
C CONTINUUM REGION FLOW OF A HIGHLY UNDEREXPANDED AXISYMMETRIC RING JET.
C RESULTS FOR THE CONTINUUM FLOW MAY BE OBTAINED FROM 'AXSYM' PROGRAM
C WHICH GIVES THE 'METHOD OF CHARACTERISTICS' ISENTROPIC SOLUTION.
C THE BOUNDARY BETWEEN THE CONTINUUM AND MOLECULAR FLOW IS DEFINED BY
C THE BREAKDOWN PARAMETER 'P' AS PROPOSED BY G. A. BIRD.
C THE 'MOLECULAR DOMAIN' IS DIVIDED INTO POLAR DIVISIONS MAKING A SET
C OF SECTORS. EACH SECTOR IS SUBDIVIDED INTO 10 REGIONS
C NO APRIORY INFORMATION ABOUT THE GEOMETRY OF THE DIFFERENT
C REGIONS IS AVAILABLE, THEREFORE, MANUAL INTERVENTION MAY BE
C REQUIRED WHEN MOVING FROM ONE SECTOR TO THE OTHER. AN ACCEPTABLE
C GEOMETRY WILL RESULT A REASONABLE NUMBER OF SIMULATED MOLECULES.
C EACH REGION IS SUBDIVIDED INTO A NUMBER OF CELLS WITH A GEOMETRY
C DEFINED BY A POLAR MESH. A NUMBER OF MOLECULES IS SET IN EACH CELL
C PROPORTIONAL TO THE CELL VOLUME. THE BOUNDARY CONDITIONS FOR EACH
C REGION REQUIRE INPUT AND OUTPUT FLUX OF MOLECULES. NO APRIORY
C INFORMATION ON THE FLUX IS AVAILABLE. IT WILL BE CALCULATED IN
C AN ITERATIVE MODE.
C IF THE BOUNDARY CONDITIONS FOR ALL CELLS ARE CONSTANT THE NUMBER
C FLUX INTO EACH CELL IS PROPORTIONAL TO CELL WALL AREA.
C TO DECREASE THE ERROR WHEN INTRODUCING MOLECULES -(INTEGER NUMBER)-
C DUE TO THE INPUT FLUX -(REAL NUMBER), AN ADDITIONAL MOLECULE IS
C GENERATED ON THE BASIS OF RANDOM NUMBERS SUCH THAT THE AVERAGE OF A
C LARGE NUMBER OF SAMPLINGS WILL EQUAL THE REAL INPUT FLUX.
C*****
C      THE MONTE CARLO SIMULATION
C THE JET GAS IS COMPOSED OF TWO SPECIES OF MOLECULES
C AMBIENT GAS IS REGARDED AS ONE SPECIES
C THE MOLECULAR MODEL IS - 'HARD SPHERE MOLECULE'
C NETWORK DEFINITION
C THE MAXIMUM RADIUS (POLAR) OF THE DOMAIN IS ASSUMED TO BE RP=15 M.
C THE ANGLE OF THE BOUNDARY BETWEEN CONTINUUM AND MOLECULAR FLOW
C AND THE SOLID WALL IS
C      ALFA (CALCULATED IN PROGRAM 'AXSYM')
C DEFINE A POLAR SECTOR WITH A RADIUS 'RP' AND AN ANGLE OF
C      DALFA =5*MFP*NAD/RP
C THIS SECTOR IS SUBDIVIDED INTO A NUMBER OF RADIAL DIVISIONS
C MAKING 'N' REGIONS FOR SIMULATION CALCULATIONS FOR EACH 'DALFA'.
C EACH REGION IS DEVIDED INTO
C      NAD -ANGULAR DIVISIONS (15) WITH AN ANGLE OF DDALFA=5*MFP/RP
C      NRD -RADIAL DIVISIONS (10)
C      MAKING NAD*NRD CELLS
C THE SMALLEST CELL CONTAINS 'MIN' MOLECULES
C      MIN = 15
C TOTAL NUMBER OF ACTIVE MOLECULES IN A REGION IS LIMITED TO 6000
C (3000 MOLECULES OF EACH SPECIES.)
C THE WIDTH OF A CELL DEFINED BY ANGLE 'DFI' MAY NOW BE EVALUATED.
C (MIN/NUMBER DENSITY = ACTUAL CELL VOLUME)
C*****
C      DEFINE PARAMETERS.....BLOCK 1
C      COMMON IX
C      DIMENSION P1(5,3000),P2(5,3000),IP(6000),C(20,10,15),
C      *IC(4,10,15),REG(5,10,20)
C      DIMENSION DFI(10),DN(10)
C      DIMENSION R(10),A(10),VOL(10),M1(10),F1(10),F2(10)
C      DIMENSION SS(2,10,10)
C      DIMENSION FEN1(4,10),FWN1(4,10),FNN1(4,15,10),FSN1(4,15,10)
C      DIMENSION FEN2(4,10),FWN2(4,10),FNN2(4,15,10),FSN2(4,15,10)
C      DIMENSION FWP1(4,10,10),FWP2(4,10,10)
C      DIMENSION FOE1(4,10,10,20),FOW1(4,10,10,20)
C      DIMENSION FOE2(4,10,10,20),FOW2(4,10,10,20)
C      DIMENSION NM(3),VRC(3),TOC(3,3),SPEC(3,5),NCOL(10,15)
C P1,P2,P3 CONTAIN INFORMATION ON UP TO M SIMULATED MOLECULES
C P1(1,N),P1(2,N),P1(3,N) ARE U,V,W VELOCITY COMPONENTS (CARTESIAN)
C P1(4,N),P1(5,N) ARE R AND TETA COORDINATES (POLAR)
C IP(M) ARE THE M MOLECULES ARRANGED IN THE ORDER OF THEIR CELLS
C C(20,I,J) CONTAINS INFORMATION ON UP TO I*J CELLS
C*****
C ALFA IS THE ANGLE WHERE THE BREAKDOWN PARAMETER EQUALS .05

```

```

C FPM IS THE MEAN FREE PATH AT ALFA. SIM00730
C***** SIM00740
C SET GENERAL CONSTANTS.....BLOCK 2 SIM00750
  IX = 529814367 SIM00760
  PI = 3.141593 SIM00770
  BOLTZ = 1.38044E-23 SIM00780
  P0 = 101325. SIM00790
  T0 = 273. SIM00800
  AVOG = 2.68699E+25 SIM00810
  RG = 8314. SIM00820
C***** SIM00830
C SET PROGRAM CONSTANTS.....BLOCK 3 SIM00840
  ISPEC=2 SIM00850
  R1 = 2.5 SIM00860
  DR=.15 SIM00870
  RP=15. SIM00880
C NUMBER OF SIMULATED MOLECULES IN SMALLEST CELL (DIFFERENT SPECIES) SIM00890
  NMOL1=3000 SIM00900
  NMOL2=3000 SIM00910
  NMOL3=0 SIM00920
  MIN = 15 SIM00930
  N1M = 15 SIM00940
  N2M = 15 SIM00950
C NUMBER OF DIVISIONS IN A SIMULATED REGION SIM00960
  NAD = 15 SIM00970
  NRDS=10 SIM00980
  NRD=10 SIM00990
  NRD1= 3 SIM01000
  NIS =2 SIM01010
C R1 IS THE RADIUS OF THE CYLINDER (WALL) SIM01020
C R(I) IS THE RADIAL COORDINATE OF CELL(I) SIM01030
C VOL(I) IS THE RATIO BETWEEN VOLUMES OF CELL(I) AND CELL(1) SIM01040
C A(I) IS THE RATIO BETWEEN INPUT FLOW AREAS OF CELL(I) AND CELL(1) SIM01050
C DR IS THE RADIAL SIZE OF A CELL (RADIAL INCREMENT) SIM01060
C INPUT THE FOLLOWING AS 'DATA' OR 'READ' STATEMENTS ***** SIM01070
  TETA = 1.2 SIM01080
C TETA IS THE FLOW DIRECTION (RADIAN) ON THE BREAKDOWN LINE AS FOUND SIM01090
C FROM THE AXSYM PROGRAM. V0 IS THE FLOW VELOCITY (M/SEC) SIM01100
  V0 = 2100 SIM01110
  VOX = V0*COS(TETA) SIM01120
  VOY = V0*SIN(TETA) SIM01130
  TWALL=300. SIM01140
  DN01=1.1E21 SIM01150
  DN02=1.1E21 SIM01160
  DTM=1.5E-6 SIM01170
C SET DATA FOR THE DIFFERENT SPECIES SIM01180
C MOLECULAR MASS SIM01190
  SPEC(1,1)=4./AVOG SIM01200
  SPEC(2,1)=40./AVOG SIM01210
  SPEC(3,1)=29./AVOG SIM01220
C MOLECULAR DIAMETER SIM01230
  SPEC(1,2)=2.19E-10 SIM01240
  SPEC(2,2)=4.00E-10 SIM01250
C SPEC(3,2)= SIM01260
C SPEC(1,3)= SIM01270
C SPEC(2,3)= ADDITIONAL DATA IF REQUIRED SIM01280
C SPEC(3,3)= SIM01290
C***** SIM01300
C THERMAL VELOCITIES AT WALL TEMPERATURE SIM01310
  VWM1=SQRT(2.*BOLTZ*TWALL/SPEC(1,1)) SIM01320
  VWM2=SQRT(2.*BOLTZ*TWALL/SPEC(2,1)) SIM01330
C SIM01340
C***** SIM01350
C INITIALISATION..RESET ALL SAMPLING VARIABLES SIM01360
  DO 80 I=1,NRD SIM01370
  DO 80 JR=1,10 SIM01380
  DO 80 JS=1,20 SIM01390
  DO 80 KPAR=1,4 SIM01400
  FOE1(KPAR,I,JR,JS)=0. SIM01410
  FOE2(KPAR,I,JR,JS)=0. SIM01420
  FOW1(KPAR,I,JR,JS)=0. SIM01430
  80 FOW2(KPAR,I,JR,JS)=0. SIM01440

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C*****SIM01450
C SET INPUT PARAMETERS.....BLOCK 3 SIM01460
  ITER=1 SIM01470
C RETURN TO 3000 FOR ADDITIONAL ITERATIONS SIM01480
  3000 KS=1 SIM01490
    ALFA=1.3 SIM01500
    FPM=.001 SIM01510
    TEMP=40. SIM01520
    VTER1=SQRT(2.*BOLTZ*TEMP/SPEC(1,1)) SIM01530
    VTER2=SQRT(2.*BOLTZ*TEMP/SPEC(2,1)) SIM01540
    IF (ITER.GT.1)GO TO 2005 SIM01550
    DO 2001 I=1,10 SIM01560
      REG(2,I,1)=DN01 SIM01570
      REG(3,I,1)=DN02 SIM01580
      DO 2001 J=1,10 SIM01590
        FWP1(2,I,J)=VOX SIM01600
        FWP2(2,I,J)=VOX SIM01610
        FWP1(3,I,J)=VOY SIM01620
        FWP2(3,I,J)=VOY SIM01630
        FWP1(4,I,J)=TEMP SIM01640
        2001 FWP2(4,I,J)=TEMP SIM01650
      2005 CONTINUE SIM01660
    C SIM01670
  C*****SIM01680
  C SIM01690
  C*****SIM01700
C DEFINE SECTOR GEOMETRY.....BLOCK 4 SIM01710
C KR IS THE INDEX FOR A REGION IN ONE SECTOR SIM01720
C RETURN TO 1000 FOR NEXT SECTOR SIM01730
  DALFA=0. SIM01740
  1000 KR=1 SIM01750
C RESET SAMPLING OF FLOW VARIABLES (N AND S) SIM01760
  DO 81 I=1,NAD SIM01770
    DO 81 JR=1,10 SIM01780
      DO 81 KPAR=1,4 SIM01790
        FNN1(KPAR,I,JR)=0. SIM01800
        FNN2(KPAR,I,JR)=0. SIM01810
        FSN1(KPAR,I,JR)=0. SIM01820
        81 FSN2(KPAR,I,JR)=0. SIM01830
  C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA SIM01840
  C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA. SIM01850
    ALFA=ALFA-DALFA SIM01860
    DALFA = 5.*FPM*FLOAT(NAD)/RP SIM01870
  C DALFA IS THE ANGLE OF THE SECTOR SIM01880
    IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2. SIM01890
    IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA SIM01900
    IF(ALFA.LE.0.)GO TO 2000 SIM01910
    DDALFA = DALFA/FLOAT(NAD) SIM01920
  C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR SIM01930
    ALFAJ=ALFA-DALFA/2. SIM01940
  C SIM01950
  C*****SIM01960
C DEFINE REGION KR IN SECTOR.....BLOCK 5 SIM01970
C RETURN TO 2000 FOR THE NEXT REGION KR SIM01980
  2000 CONTINUE SIM01990
C RESET SAMPLING OF FLOW VARIABLES PER REGION SIM02000
  DO 82 I=1,NRD SIM02010
    DO 82 KPAR=1,4 SIM02020
      FEN1(KPAR,I)=0. SIM02030
      FEN2(KPAR,I)=0. SIM02040
      FWN1(KPAR,I)=0. SIM02050
      82 FWN2(KPAR,I)=0. SIM02060
    MT=0 SIM02070
    NRD=NRDS SIM02080
    IF(KR.LT.2)NRD=NRD1 SIM02090
    DO 100 I = 1,NRD SIM02100
  C POLAR RADIUS MEASURED FROM THE NOZZLE LIP SIM02110
    R(I) =(FLOAT(I)-.5)*DR SIM02120
    IF(KR.EQ.2)R(I)=R(I)+FLOAT(NRD1)*DR SIM02130
    IF(KR.GE.3)R(I)=R(I)+(FLOAT(NRD1+(KR-2)*NRD))*DR SIM02140
  C RSI IS THE RADIUS MEASURED FROM THE AXIS OF SYMMETRY SIM02150
    RSI=R(I)+R1/SIN(ALFAJ) SIM02160

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      IF(I.EQ.1)RS1=RSI
      A(I) = RSI/RS1
      VOL(I) = R(I)*RSI/(R(1)*RS1)
      M1(I) = MIN*VOL(I)
      MT = MT+M1(I)
C M1(I) IS THE INITIAL NUMBER OF MOLECULES IN EACH CELL
      DN1=REG(2,KR,KS)
      DN2=REG(3,KR,KS)
      REG(1,KR,KS)=FLOAT(MIN)/(DN1*R(1)*RS1*DR*DDALFA)
C DFI (REG(1,KR,KS)) IS THE SPHERICAL (AXISYMMETRIC) ANGLE
C THIS ANGLE HAS DIFFERENT VALUES FOR EACH KR, THEREFORE IT IS A
C WEIGHTING FACTOR.++++++++++++++++++++++++++++++++++++++++
C (FNN1,FNN2,FSN1,FSN2,FEN1,FEN2,FWN1,FWN2) * DFI
C (FOE1,FOE2,FOW1,FOW2) * DFI
      DA1 = RS1*DR*REG(1,KR,KS)
C DA1 IS THE INPUT AREA OF CELL(I)
      FN1 = V0*DA1*REG(2,KR,KS)*SIN(ALFA-TETA)
      FN2 = V0*DA1*REG(3,KR,KS)*SIN(ALFA-TETA)
C TETA IS THE ANGLE BETWEEN FLOW DIRECTION AND THE WALL
      F1(I) = FN1*A(I)
      F2(I) = FN2*A(I)
C
      99 FWP1(1,I,KR)=F1(I)
      100 FWP2(1,I,KR)=F2(I)
C
C .....
C DEFINE ACTUAL VOLUME AND INPUT AREA OF SMALLEST CELL IN REGION
      REG(4,KR,KS)=R(1)*DDALFA*DR*RS1*REG(1,KR,KS)
      REG(5,KR,KS)=DA1
C FN1 IS THE NUMBER FLUX TO THE SMALLEST CELL (REAL NUMBER) PER SECOND.
C INPUT NUMBER OF MOLECULES (INTEGER) WILL BE INTEGRATED TO MAKE AN
C AVERAGE OF FN1.
C F1(I) IS THE INPUT FLUX TO CELL(I)
C FOLLOWING ARE THE REGION BOUNDARIES
      102 RMIN=R(1)-.5*DR
      RMAX=RMIN+DR*FLOAT(NRD)
      TMAX=ALFA
      TMIN=ALFA-DALFA
      DO 9102 I = 1,NRD
      WRITE (6,9101)R(I),A(I),VOL(I),M1(I),F1(I)
9101 FORMAT(' ',3F13.5,I10,E15.5)
9102 CONTINUE
      MTT= MT*NAD
      WRITE(6,103)MT,MTT
      103 FORMAT (' INITIAL NUMBER OF SIMULATED MOLECULES IS= ',I5,' PER SPESIM02600
      XCIES PER DDALFA, TOTAL NUMBER IS', I5) SIM02610
C*****SIM02620
C DEFINE INPUT FLOWS TO KR W,E,N,S.....BLOCK 6 SIM02630
C
C
C
C*****SIM02670
C CALCULATE INITIAL NUMBER OF MOLECULES IN CELLS.....BLOCK 7 SIM02680
C SET INITIAL STATE OF GAS.....' ' 8 SIM02690
C
      DO 150 I =1,NRD
      DO 150 J= 1,NAD
      SIM02700
      SIM02710
      SIM02720
      SIM02730
      SIM02740
      SIM02750
      SIM02760
      SIM02770
      SIM02780
      SIM02790
      SIM02800
      SIM02810
      SIM02820
      SIM02830
      SIM02840
      SIM02850
      SIM02860
      SIM02870
      SIM02880
C
C DEACTIVATE ALL MOLECULES
      DO 170 N = 1,NMOLL
      P1(4,N) = -99.
      170 P2(4,N) = -99.

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C		SIM02890
C	*****	SIM02900
C	SET INITIAL STATE OF THE GAS (LOCATION AND VELOCITY OF MOLECULES)	SIM02910
C		SIM02920
	NADR1 = 0	SIM02930
	NADR2 = 0	SIM02940
	DO 200 I = 1,NRD	SIM02950
	DO 200 J = 1,NAD	SIM02960
	NM1 = IC(1,I,J)	SIM02970
C		SIM02980
	DO 205 N = 1,NM1	SIM02990
	NADR1 = NADR1 + 1	SIM03000
	CALL RANDU(PP)	SIM03010
	P1(4,NADR1) = C(19,I,J)+DR*(PP-.5)	SIM03020
	CALL RANDU(P)	SIM03030
	P1(5,NADR1) = C(20,I,J)+DDALFA*(P-.5)	SIM03040
C		SIM03050
	DO 205 NV = 1,3	SIM03060
203	CALL RANDU(P)	SIM03070
	V = -3.+6.*P	SIM03080
	B = EXP(-V*V)	SIM03090
	CALL RANDU(P)	SIM03100
	IF(B.LT.P) GO TO 203	SIM03110
	P1(NV,NADR1) = P*SIN(B)*VTER1	SIM03120
	IF(NV.EQ.1)P1(NV,NADR1)=P1(NV,NADR1)+V0X	SIM03130
	IF(NV.EQ.2)P1(NV,NADR1)=P1(NV,NADR1)+V0Y	SIM03140
205	CONTINUE	SIM03150
C		SIM03160
C	REPEAT PROCEDURE FOR SPECIES 2	SIM03170
	NM2 = IC(2,I,J)	SIM03180
	DO 210 N = 1,NM2	SIM03190
	NADR2 = NADR2+1	SIM03200
	CALL RANDU(P)	SIM03210
	P2(4,NADR2) = C(19,I,J)+DR*(P-.5)	SIM03220
	CALL RANDU(P)	SIM03230
	P2(5,NADR2) = C(20,I,J)+DDALFA*(P-.5)	SIM03240
C		SIM03250
	DO 210 NV = 1,3	SIM03260
207	CALL RANDU(P)	SIM03270
	V = -3.+6.*P	SIM03280
	B = EXP(-V*V)	SIM03290
	CALL RANDU(P)	SIM03300
	IF(B.LT.P) GO TO 207	SIM03310
	P2(NV,NADR2) = P*SIN(B)*VTER2	SIM03320
	IF(NV.EQ.1)P2(NV,NADR2)=P2(NV,NADR2)+V0X	SIM03330
	IF(NV.EQ.2)P2(NV,NADR2)=P2(NV,NADR2)+V0Y	SIM03340
210	CONTINUE	SIM03350
C		SIM03360
C	WHEN NECESSARY, REPEAT PROCEDURE FOR SPECIES 3.	SIM03370
	200 CONTINUE	SIM03380
C		SIM03390
C	*****	SIM03400
C	DEFINE HERE ALL COLLISION PARAMETERS TO BE INCLUDED IN SIMULATION	SIM03410
C		BLOCK 9
C	RESET COLLISION TIMERS	SIM03420
	DO 19 I=1,NRD	SIM03430
	DO 19 J=1,NAD	SIM03440
	DO 19 L=1,3	SIM03450
	DO 19M=1,3	SIM03460
	KT=3*(L-1)+M+9	SIM03470
	C(KT,I,J)=0.	SIM03480
C	SET EXPECTED MAXIMUM RELATIVE VELOCITY IN COLLISIONS	SIM03490
	KV=3*(L-1)+M	SIM03500
	EM1=SPEC(L,1)	SIM03510
	EM2=SPEC(M,1)	SIM03520
	EMR=EM1*EM2/(EM1+EM2)	SIM03530
C		SIM03540
	IF(KS.EQ.1)GO TO 17	SIM03550
	TEM=FOE1(4,I,KR,KS)	SIM03560
	GO TO 18	SIM03570
17	TEM=FWP1(4,I,KR)	SIM03580
C		SIM03590
		SIM03600

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18 RV=2./SQRT(PI*2.*BOLTZ*TEM/EMR)
19 C(KV,I,J)=2.*RV
C
C MAXIMUM RELATIVE VELOCITY WILL BE RESET IF FASTER ENCOUNTERS OCCUR
C
C *****
C TIME=0.
C LOOP OVER TIME INTERVALS.....BLOCK 10
  DO 6000 JDTM = 1,NIS
C
C
C TIME=TIME+DTM
C *****
C MOVE ALL MOLECULES .....BLOCK 12
C MOVE MOLECULES OF SPECIES 1
C
  DO 310 I1 = 1,NMOL1
C SKIP INACTIVE MOLECULES.....13
  IF (P1(4,I1).EQ.-99.) GO TO 310
  VX = P1(1,I1)
  VY = P1(2,I1)
  RX = P1(4,I1)
  T = P1(5,I1)
  TOLD=T
C *****
C FIND NEW COORDINATES.....BLOCK 14
  XX=RX*COS(T)+VX*DTM
  YY=RX*SIN(T)+VY*DTM
  RNEW=SQRT(XX**2+YY**2)
  T=ATAN(YY/XX)
C *****
C FOR LAST SECTOR FIND COLLISIONS WITH THE WALL AND SAMPLE THEM
C .....BLOCK 15,16
  IF(ALFA.GT.DALFA)GO TO 301
  IF(T.GT.0.)GO TO 301
  DTR=DTM*T/(T-TOLD)
C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL
  IF(DTR.LT.1E-10)DTR=1E-10
  RW=RX+(RNEW-RX)*DTR/DTM
  IF(RW.LT.RMIN)RW=RMIN+DTR*.001
  IF(RW.GT.RMAX)RW=RMAX-DTR*.001
  LOC=RW/DR+1.
C
C COUNT COLLISIONS WITH THE WALL(MUST BE WAIGHTED =*DFI)
  SS(1,LOC,JSAMP)=SS(1,LOC,JSAMP)+1
C
C SET VELOCITY AND LOCATION AFTER A MOLECULE STRIKES THE WALL
302 CALL RANDU(P)
  B=VWM1*SQRT(-ALOG(P))
  CALL RANDU(P)
  BB=2.*PI*P
  P1(1,NADRI)=B*COS(BB)
  VX=B*COS(BB)
  P1(2,NADRI)=B*SIN(BB)
  VY=B*SIN(BB)
  CALL RANDU(P)
  P1(3,NADRI)=VWM1*SQRT(-ALOG(P))
  XX=RX*COS(T)+VX*DTR
  YY=RX*SIN(T)+VY*DTR
  RNEW=SQRT(XX**2+YY**2)
  T=ATAN(YY/XX)
C
C *****
C DEACTIVATE ALL MOLECULES THAT MOVED OUT.....BLOCK 17
301 IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN.AND.T.LT.TMAX.AND.T.GT.TMIN)GO TO
  *303
  RI=(RNEW-RMIN)/DR+.999999
  IR=RI
  TI=(TMAX-T)/DDALFA+.999999
  IT=TI
C

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SIM03610
SIM03620
SIM03630
SIM03640
SIM03650
SIM03660
SIM03670
SIM03680
SIM03690
SIM03700
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SIM03990
SIM04000
SIM04010
SIM04020
SIM04030
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SIM04070
SIM04080
SIM04090
SIM04100
SIM04110
SIM04120
SIM04130
SIM04140
SIM04150
SIM04160
SIM04170
SIM04180
SIM04190
SIM04200
SIM04210
SIM04220
SIM04230
SIM04240
SIM04250
SIM04260
SIM04270
SIM04280
SIM04290
SIM04300
SIM04310
SIM04320

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IF(IT.LE.0)GO TO 304	SIM04330
IF(IT.GT.NAD)GO TO 305	SIM04340
IF(IR.GT.NRD)GO TO 306	SIM04350
C COUNT S DIRECTION, SAMPLE.....18	SIM04360
FSN1(1,IT,KR)=FSN1(1,IT,KR)+1.	SIM04370
GO TO 309	SIM04380
C COUNT W DIRECTION, SAMPLE.....18	SIM04390
304 IF(IR.LE.0)IR=1	SIM04400
IF(IR.GT.NRD)IR=NRD	SIM04410
FWN1(1,IR)=FWN1(1,IR)+1.	SIM04420
GO TO 309	SIM04430
C COUNT E DIRECTION, SAMPLE.....18	SIM04440
305 IF(IR.LE.0)IR=1	SIM04450
IF(IR.GT.NRD)IR=NRD	SIM04460
FEN1(1,IR)=FEN1(1,IR)+1.	SIM04470
GO TO 309	SIM04480
C COUNT N DIRECTION, SAMPLE.....18	SIM04490
306 FNN1(1,IT,KR)=FNN1(1,IT,KR)+1.	SIM04500
C SET NEW VALUES IN THE MOLECULE TABLE	SIM04510
C	SIM04520
309 RNEW=-99.	SIM04530
303 P1(4,I1)=RNEW	SIM04540
P1(5,I1)=T	SIM04550
310 CONTINUE	SIM04560
C	SIM04570
C	SIM04580
C REPEAT PROCEDURE FOR SPECIES 2 MOLECULES.....BLOCKS 12 TO18	SIM04590
DO 320 I2=1,NMOL2	SIM04600
C SKIP INACTIVE MOLECULES	SIM04610
IF(P2(4,I2).EQ.-99.)GO TO 320	SIM04620
VX = P2(1,I2)	SIM04630
VY = P2(2,I2)	SIM04640
RX = P2(4,I2)	SIM04650
T = P2(5,I2)	SIM04660
TOLD=T	SIM04670
C	SIM04680
XX=RX*COS(T)+VX*DTM	SIM04690
YY=RX*SIN(T)+VY*DTM	SIM04700
RNEW=SQRT(XX**2+YY**2)	SIM04710
T=ATAN(YY/XX)	SIM04720
C COLLISIONS WITH THE WALL	SIM04730
C	SIM04740
IF(ALFA.GT.DALFA)GO TO 311	SIM04750
IF(T.GT.0.)GO TO 311	SIM04760
DTR=DTM*T/(T-TOLD)	SIM04770
C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL	SIM04780
IF(DTR.LT.1E-10)DTR=1E-10	SIM04790
RW=RX+(RNEW-RX)*DTR/DTM	SIM04800
IF(RW.LT.RMIN)RW=RW+DTR*.001	SIM04810
IF(RW.GT.RMAX)RW=RW-DTR*.001	SIM04820
LOC=RW/DR+1	SIM04830
C COUNT COLLISIONS WITH THE WALL (MUST BE WEIGHTED =*DFI)	SIM04840
SS(2,LOC,JSAMP)=SS(2,LOC,JSAMP)+1	SIM04850
C	SIM04860
C FIND THE NEW COORDINATES OF THE MOLECULE	SIM04870
312 CALL RANDU(P)	SIM04880
B=VWM2*SQRT(-ALOG(P))	SIM04890
CALL RANDU(P)	SIM04900
BB=2.*PI*P	SIM04910
P2(1,NADR2)=B*COS(BB)	SIM04920
VX=B*COS(BB)	SIM04930
P2(2,NADR2)=B*SIN(BB)	SIM04940
VY=B*SIN(BB)	SIM04950
CALL RANDU(P)	SIM04960
XX=RX*COS(T)+VX*DTR	SIM04970
YY=RX*SIN(T)+VY*DTR	SIM04980
RNEW=SQRT(XX**2+YY**2)	SIM04990
T=ATAN(YY/XX)	SIM05000
C	SIM05010
C DEACTIVATE MOLECULES THAT MOVED OUT.COUNT FOR OUTPUT FLUX EVALUATION.	SIM05020
311 IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN.AND.T.LT.TMAX.AND.T.GT.TMIN)GO TO	SIM05030
*313	SIM05040

RI = (RNEW-RMIN)/DR+.999999	SIM05050
IR = RI	SIM05060
TI = (TMAX-T)/DDALFA+.999999	SIM05070
IT = TI	SIM05080
IF (IT.LE.0)GO TO 314	SIM05090
IF (IT.GT.NAD)GO TO 315	SIM05100
IF(IR.GT.NRD)GO TO 316	SIM05110
C COUNT S DIRECTION, SAMPLE.....18	SIM05120
FSN2(1,IT,KR)=FSN2(1,IT,KR)+1.	SIM05130
GO TO 319	SIM05140
C COUNT W DIRECTION, SAMPLE.....18	SIM05150
314 IF(IR.LE.0)IR=1	SIM05160
IF(IR.GT.NRD)IR=NRD	SIM05170
FWN2(1,IR)=FWN2(1,IR)+1.	SIM05180
GO TO 319	SIM05190
C COUNT E DIRECTION, SAMPLE.....18	SIM05200
315 IF(IR.LE.0)IR=1	SIM05210
IF(IR.GT.NRD)IR=NRD	SIM05220
FEN2(1,IR)=FEN2(1,IR)+1.	SIM05230
GO TO 319	SIM05240
C COUNT N DIRECTION, SAMPLE,.....18	SIM05250
316 FNN2(1,IT,KR)=FNN2(1,IT,KR)+1.	SIM05260
C	SIM05270
319 RNEW = -99.	SIM05280
C.....19	SIM05290
313 P2(4,I2)= RNEW	SIM05300
P2(5,I2)= T	SIM05310
320 CONTINUE	SIM05320
C	SIM05330
C*****	SIM05340
C NOW NEW MOLECULES WILL BE INTRODUCED	SIM05350
C TOTAL JET FLUX INTO THE REGION WAS DETERMINED BY F1(I) MOL./SEC.	SIM05360
C OR FWP1(I,KR),FWP2(I,KR) FOR EACH SPECIES	SIM05370
C NUMBER OF MOLECULES TO BE ACTIVATED PER DTM IS F(I)*DTM PER CELL.	SIM05380
C	SIM05390
C*****	SIM05400
DO 390 I=1,NRD	SIM05410
C INPUT 'W' MOLECULES	SIM05420
IF(KS.EQ.1)GO TO 322	SIM05430
ANEW1=FOE1(1,I,KR,KS-1)	SIM05440
ANEW2=FOE2(1,I,KR,KS-1)	SIM05450
GO TO 323	SIM05460
322 ANEW1=FWP1(1,I,KR)*DTM	SIM05470
ANEW2=FWP2(1,I,KR)*DTM	SIM05480
323 NEW1=ANEW1	SIM05490
NEW2=ANEW2	SIM05500
REM1=ANEW1-NEW1	SIM05510
CALL RANDU(P)	SIM05520
IF(REM1.GT.P)NEW1=NEW1+1	SIM05530
REM2=ANEW2-NEW2	SIM05540
CALL RANDU(P)	SIM05550
IF(REM2.GT.P)NEW2=NEW2+1	SIM05560
C ACTIVATE NEW INPUT MOLECULES	SIM05570
C TIME, LOCATION AND VELOCITY COMP. OF NEW MOL. ARE RANDOM FUNCTIONS	SIM05580
C SPECIES 1.....	SIM05590
IF(NEW1.LT.1)GO TO 341	SIM05600
C	SIM05610
DO 340 I1=1,NEW1	SIM05620
CALL RANDU(P)	SIM05630
ATIME=P*DTM	SIM05640
CALL RANDU(P)	SIM05650
RSTART=(FLOAT(I-1)+P)*DR+RMIN	SIM05660
VELX=FWP1(2,I,KR)	SIM05670
VELY=FWP1(3,I,KR)	SIM05680
TEM=FWP1(4,I,KR)	SIM05690
C THERMAL VELOCITY	SIM05700
VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))	SIM05710
C TEMPERATURE IS TRANSFERRED THROUGH FWP1(4,I,KR)	SIM05720
XX=RSTART*COS(ALFA)+VELX*ATIME	SIM05730
YY=RSTART*SIN(ALFA)+VELY*ATIME	SIM05740
RX=SQRT(XX**2+YY**2)	SIM05750
T=ATAN(YY/XX)	SIM05760

IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 340	SIM05770
IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 340	SIM05780
C FOR MORE ACCURATE CALCULATION SET THESE MOLECULES IN OUTPUT FLOWS	SIM05790
C	SIM05800
C DEFINE THE VELOCITY COMPONENTS	SIM05810
CALL RANDU(P)	SIM05820
B=VTER1*SQRT(-ALOG(P))	SIM05830
CALL RANDU(P)	SIM05840
BB=2.*PI*P	SIM05850
VELX=VELX+B*COS(BB)	SIM05860
VELY=VELY+B*SIN(BB)	SIM05870
CALL RANDU(P)	SIM05880
VELZ=VTER1*SQRT(-ALOG(P))	SIM05890
C DEFINE THE NEW MOLECULE TO BE ACTIVATED	SIM05900
DO 325 IACT=1,NMOL1	SIM05910
IF(P1(4,IACT).EQ.-99.)GO TO 326	SIM05920
325 CONTINUE	SIM05930
C	SIM05940
C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE PRINT 'ALARM'	SIM05950
IF(IACT.GE.NMOL1)GO TO 3004	SIM05960
326 P1(4,IACT)=RX	SIM05970
P1(5,IACT)=T	SIM05980
P1(1,IACT)=VELX	SIM05990
P1(2,IACT)=VELY	SIM06000
P1(3,IACT)=VELZ	SIM06010
340 CONTINUE	SIM06020
C	SIM06030
C REPEAT PROCEDURE FOR SPECIES 2	SIM06040
341 IF(NEW2.LT.1)GO TO 351	SIM06050
DO 350 I2=1,NEW2	SIM06060
CALL RANDU(P)	SIM06070
ATIME=P*DTM	SIM06080
CALL RANDU(P)	SIM06090
RSTART=RMIN+(FLOAT(I-1)+P)*DR	SIM06100
VELX=FWP2(2,I,KR)	SIM06110
VELY=FWP2(3,I,KR)	SIM06120
TEM=FWP2(4,I,KR)	SIM06130
C THERMAL VELOCITY	SIM06140
VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))	SIM06150
XX=RSTART*COS(ALFA)+VELX*ATIME	SIM06160
YY=RSTART*SIN(ALFA)+VELY*ATIME	SIM06170
RX=SQRT(XX**2+YY**2)	SIM06180
T=ATAN(YY/XX)	SIM06190
IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 350	SIM06200
IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 350	SIM06210
C FOR MORE ACCURATE RESULTS SET THESE MOLECULES IN OUTPUT FLOWS	SIM06220
C	SIM06230
C DEFINE VELOCITY COMPONENTS	SIM06240
CALL RANDU(P)	SIM06250
B=VTER2*SQRT(-ALOG(P))	SIM06260
CALL RANDU(P)	SIM06270
BB=2.*PI*P	SIM06280
VELX=VELX+B*COS(BB)	SIM06290
VELY=VELY+B*SIN(BB)	SIM06300
CALL RANDU(P)	SIM06310
VELZ=VTER2*SQRT(-ALOG(P))	SIM06320
C FIND A NEW MOLECULE TO BE ACTIVATED	SIM06330
DO 345 IACT=1,NMOL2	SIM06340
IF (P2(4,IACT).EQ.-99.)GO TO 346	SIM06350
345 CONTINUE	SIM06360
C IF THERE IS NO PLACE THEN PRINT ALARM	SIM06370
IF(IACT.EQ.NMOL2)GO TO 3004	SIM06380
346 P2(4,IACT)=RX	SIM06390
P2(5,IACT)=T	SIM06400
P2(1,IACT)=VELX	SIM06410
P2(2,IACT)=VELY	SIM06420
P2(3,IACT)=VELZ	SIM06430
350 CONTINUE	SIM06440
C	SIM06450
C REPEAT PROCEDURE FOR SPEC-3	SIM06460
C	SIM06470
C INPUT E MOLECULES	SIM06480

P2(5,IACT)=T	SIM07210
P2(1,IACT)=VELX	SIM07220
P2(2,IACT)=VELY	SIM07230
382 P2(3,IACT)=VELZ	SIM07240
C.....	SIM07250
C REPEAT FOR SPEC-3	SIM07260
C	SIM07270
390 CONTINUE	SIM07280
C.....	SIM07290
C INPUT 'S' MOLECULES	SIM07300
DO 460 J=1,NAD	SIM07310
IF(KR.LT.2)GO TO 460	SIM07320
ANEW1=FNN1(1,J,KR-1)	SIM07330
IF(ANEW1.LE..00001)GO TO 420	SIM07340
NEW1=ANEW1	SIM07350
REM=ANEW1-NEW1	SIM07360
CALL RANDU(P)	SIM07370
IF(P.LT.REM)NEW1=NEW1+1	SIM07380
DO 402 I1=1,NEW1	SIM07390
CALL RANDU(P)	SIM07400
T=TMIN+DDALFA*(P+FLOAT(J-1))	SIM07410
CALL RANDU(P)	SIM07420
RNEW=RMIN+P*DR	SIM07430
CALL RANDU(P)	SIM07440
TEM=FNN1(4,J,KR-1)	SIM07450
VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))	SIM07460
B=VTER1*SQRT(-ALOG(P))	SIM07470
CALL RANDU(P)	SIM07480
BB=2.*PI*P	SIM07490
VELX=FNN1(2,J,KR-1)+B*COS(BB)	SIM07500
VELY=FNN1(3,J,KR-1)+B*SIN(BB)	SIM07510
CALL RANDU(P)	SIM07520
VELZ=VTER1*SQRT(-ALOG(P))	SIM07530
C FIND A NEW MOLECULE TO BE ACTIVATED	SIM07540
DO 404 IACT=1,NMOL1	SIM07550
IF(P1(4,IACT).EQ.-99.)GO TO 406	SIM07560
404 CONTINUE	SIM07570
IF(IACT.EQ.NMOL1)GO TO 3004	SIM07580
406 P1(4,IACT)=RNEW	SIM07590
P1(5,IACT)=T	SIM07600
P1(1,IACT)=VELX	SIM07610
P1(2,IACT)=VELY	SIM07620
402 P1(3,IACT)=VELZ	SIM07630
420 CONTINUE	SIM07640
C REPEAT FOR SPECIES 2	SIM07650
ANEW2=FNN2(1,J,KR-1)	SIM07660
IF(ANEW2.LT..00001)GO TO 440	SIM07670
NEW2=ANEW2	SIM07680
REM=ANEW2-NEW2	SIM07690
CALL RANDU(P)	SIM07700
IF(P.LT.REM)NEW2=NEW2+1	SIM07710
DO 422 I2=1,NEW2	SIM07720
CALL RANDU(P)	SIM07730
T=TMIN+DDALFA*(P+FLOAT(J-1))	SIM07740
CALL RANDU(P)	SIM07750
RNEW=RMIN+P*DR	SIM07760
CALL RANDU(P)	SIM07770
TEM=FNN2(4,J,KR-1)	SIM07780
VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))	SIM07790
B=VTER2*SQRT(-ALOG(P))	SIM07800
CALL RANDU(P)	SIM07810
BB=2.*PI*P	SIM07820
VELX=FNN2(2,J,KR-1)+B*COS(BB)	SIM07830
VELY=FNN2(3,J,KR-1)+B*SIN(BB)	SIM07840
CALL RANDU(P)	SIM07850
VELZ=VTER2*SQRT(-ALOG(P))	SIM07860
C FIND A NEW MOLECULE TO BE ACTIVATED	SIM07870
DO 424 IACT=1,NMOL2	SIM07880
IF(P2(4,IACT).EQ.-99)GO TO 426	SIM07890
424 CONTINUE	SIM07900
IF(IACT.EQ.NMOL2)GO TO 3004	SIM07910
426 P2(4,IACT)=RNEW	SIM07920

P2(5, IACT)=T	SIM07930
P2(1, IACT)=VELX	SIM07940
P2(2, IACT)=VELY	SIM07950
422 P2(3, IACT)=VELZ	SIM07960
440 CONTINUE	SIM07970
C.....	SIM07980
C REPEAT FOR SPEC-3	SIM07990
C.....	SIM08000
C INPUT 'N' MOLECULES.....	SIM08010
C SPEC-1	SIM08020
ANEW1=FSN1(1, J, KR+1)	SIM08030
IF(ANEW1.LE..00001)GO TO 450	SIM08040
NEW1=ANEW1	SIM08050
REM=ANEW1-NEW1	SIM08060
CALL RANDU(P)	SIM08070
IF (P.LT.REM)NEW1=NEW1+1	SIM08080
DO 442 I1=1, NEW1	SIM08090
CALL RANDU(P)	SIM08100
T=TMIN +DDALFA*(P+FLOAT(J-1))	SIM08110
CALL RANDU(P)	SIM08120
RNEW=RMAX-P*DR	SIM08130
CALL RANDU(P)	SIM08140
TEM=FSN1(4, J, KR+1)	SIM08150
VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))	SIM08160
B=VTER1*SQRT(-ALOG(P))	SIM08170
CALL RANDU(P)	SIM08180
BB=2.*PI*P	SIM08190
VELX=FSN1(2, J, KR+1)+B*COS(BB)	SIM08200
VELY=FSN1(3, J, KR+1)+B*SIN(BB)	SIM08210
CALL RANDU(P)	SIM08220
VELZ=VTER1*SQRT(-ALOG(P))	SIM08230
C FIND A NEW MOLECULE TO BE ACTIVATED	SIM08240
DO 444 IACT=1, NMOL1	SIM08250
IF(P1(4, IACT).EQ.-99.)GO TO 446	SIM08260
444 CONTINUE	SIM08270
IF(IACT.EQ.NMOL1)GO TO 3004	SIM08280
446 P1(4, IACT)=RNEW	SIM08290
P1(5, IACT)=T	SIM08300
P1(1, IACT)=VELX	SIM08310
P1(2, IACT)=VELY	SIM08320
442 P1(3, IACT)=VELZ	SIM08330
450 CONTINUE	SIM08340
C.....	SIM08350
C INPUT N MOLECULES SPEC-2	SIM08360
ANEW2=FSN2(1, J, KR+1)	SIM08370
IF(ANEW2.LE..00001)GO TO 460	SIM08380
NEW2=ANEW2	SIM08390
REM=ANEW2-NEW2	SIM08400
CALL RANDU(P)	SIM08410
IF(P.LT.REM)NEW2=NEW2+1	SIM08420
DO 452 I2=1, NEW2	SIM08430
CALL RANDU(P)	SIM08440
T=TMIN+DDALFA*(P+FLOAT(J-1))	SIM08450
CALL RANDU(P)	SIM08460
RNEW=RMAX-P*DR	SIM08470
CALL RANDU(P)	SIM08480
TEM=FSN2(4, J, KR+1)	SIM08490
VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))	SIM08500
B=VTER2*SQRT(-ALOG(P))	SIM08510
CALL RANDU(P)	SIM08520
BB=2*PI*P	SIM08530
VELX=FSN2(2, J, KR+1)+B*COS(BB)	SIM08540
VELY=FSN2(3, J, KR+1)+B*SIN(BB)	SIM08550
CALL RANDU(P)	SIM08560
VELZ=VTER2*SQRT(-ALOG(P))	SIM08570
C FIND A NEW MOLECULE TO BE ACTIVATED	SIM08580
DO 454 IACT=1, NMOL2	SIM08590
IF(P2(4, IACT).EQ.-99)GO TO 456	SIM08600
454 CONTINUE	SIM08610
IF(IACT.EQ.NMOL2)GO TO 3004	SIM08620
456 P2(4, IACT)=RNEW	SIM08630
P2(5, IACT)=T	SIM08640

P2(1,IACT)=VELX	SIM08650
P2(2,IACT)=VELY	SIM08660
452 P2(3,IACT)=VELZ	SIM08670
460 CONTINUE	SIM08680
	SIM08690
	SIM08700
*****	SIM08710
*****	SIM08720
REARRANGE MOLECULES IN THEIR CELLS	SIM08730
C INITIALIZATION	SIM08740
5000 CONTINUE	SIM08750
*****	SIM08760
KIP=NMOL1+NMOL2+NMOL3	SIM08770
DO 1001 KADD=1,KIP	SIM08780
1001 IP(KADD)=0	SIM08790
KADD=0	SIM08800
N1A=0	SIM08810
N2A=0	SIM08820
N3A=0	SIM08830
C N1A,N2A,N3A ARE THE NUMBER OF ACTIVE MOLECULES (COUNTED NEXT)	SIM08840
	SIM08850
DO 1100 I=1,NRD	SIM08860
DO 1100 J=1,NAD	SIM08870
	SIM08880
DO 1005 K=1,4	SIM08890
1005 IC(K,I,J)=0	SIM08900
	SIM08910
C SET SPECIES 1	SIM08920
N1C=0	SIM08930
N2C=0	SIM08940
N3C=0	SIM08950
NTC=0	SIM08960
DO 1020 K1=1,NMOL1	SIM08970
IF(P1(4,K1).EQ.-99.)GO TO 1020	SIM08980
RLOC=ABS(C(19,I,J)-P1(4,K1))	SIM08990
TLOC=ABS(C(20,I,J)-P1(5,K1))	SIM09000
IF(RLOC.GT.DR*.5)GO TO 1020	SIM09010
IF(TLOC.GT.DDALFA*.5)GO TO 1020	SIM09020
	SIM09030
N1C=N1C+1	SIM09040
NTC=NTC+1	SIM09050
N1A=N1A+1	SIM09060
IF(NTC.EQ.1)IC(4,I,J)=KADD	SIM09070
IC(1,I,J)=IC(1,I,J)+1	SIM09080
KADD=KADD+1	SIM09090
IP(KADD)=K1	SIM09100
1020 CONTINUE	SIM09110
C SET SPEC-2 MOLECULES.....	SIM09120
DO 1040 K2=1,NMOL2	SIM09130
IF(P2(4,K2).EQ.-99.)GO TO 1040	SIM09140
RLOC=ABS(C(19,I,J)-P2(4,K2))	SIM09150
TLOC=ABS(C(20,I,J)-P2(5,K2))	SIM09160
IF(RLOC.GT.DR*.5)GO TO 1040	SIM09170
IF(TLOC.GT.DDALFA*.5)GO TO 1040	SIM09180
	SIM09190
N2A=N2A+1	SIM09200
NTC=NTC+1	SIM09210
IF(NTC.EQ.1)IC(4,I,J)=KADD	SIM09220
IC(2,I,J)=IC(2,I,J)+1	SIM09230
KADD=KADD+1	SIM09240
IP(KADD)=K2	SIM09250
1040 CONTINUE	SIM09260
1100 CONTINUE	SIM09270
WRITE(6,1021)N1A,N2A	SIM09280
1021 FORMAT(' NUMBER OF ACTIVE MOLECULES SPEC1= ',I5,' SPEC2=',I5/)	SIM09290
	SIM09300
	SIM09310
*****	SIM09320
C CALCULATE COLLISIONS.....BLOCK	SIM09330
C EXTERNAL LOOPS ARE OVER CELLS I,J	SIM09340
*****	SIM09350
	SIM09360

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DO 999 I=1,NRD
DO 999 J=1,NAD
999 NCOL(I,J)=0
C
DO 900 I=1,NRD
DO 900 J=1,NAD
C
NM(1)=IC(1,I,J)
NM(2)=IC(2,I,J)
NM(3)=IC(3,I,J)
NTOT=NM(1)+NM(2)+NM(3)
DO 900 L=1,3
DO 900 M=1,3
C NUMBER OF SPECIES IN THE PROGRAM IS 2 (3)
KV=(L-1)*3+M
KT=KV+9
C KV,KT ARE THE ADDRESSES OF RELATIVE VELOCITY AND COLLISION TIMERS
920 IF(C(KT,I,J).GE.TIME) GO TO 900
C C(KT,I,J) IS THE INTEGRATED TIME FOR L-M COLLISION
KSEL=0
KREJ=0
IF(NM(L).GT.1.AND.NM(M).GT.1)GO TO 912
C NO COLLISIONS ARE CALCULATED IF THERE ARE NO MOLECULES
911 C(KT,I,J)=C(KT,I,J)+DTM
GO TO 900
C SELECT NOW THE MOLECULES FOR COLLISION
912 IF (KSEL.GE.100)GO TO 911
CALL RANDU(P)
MOL1=P*NM(L)+.999999
IF(MOL1.EQ.0)MOL1=1
C
CALL RANDU(P)
MOL2=P*NM(M)+.999999
IF(MOL2.EQ.0)MOL2=1
C
KSEL=KSEL+1
C
C CHECK IF THE SAME MOLECULE HAS BEEN SELECTED TWICE
IF(L.EQ.M.AND.MOL1.EQ.MOL2)GO TO 912
C
C FIND THE ACTUAL ADDRESSES OF THE SELECTED MOLECULES
IF(L.EQ.1)K1=0
IF(L.EQ.2)K1=NM(1)
IF(L.EQ.3)K1=NM(1)+NM(2)
IF(M.EQ.1)K2=0
IF(M.EQ.2)K2=NM(1)
IF(M.EQ.3)K2=NM(1)+NM(2)
KAD1=MOL1+K1+IC(4,I,J)
KAD2=MOL2+K2+IC(4,I,J)
C KAD1,KAD2 ARE THE LOCATION OF SELECTED MOLECULES IN IP( )
MAD1=IP(KAD1)
MAD2=IP(KAD2)
C MAD1,MAD2 ARE THE ACTUAL ADDRESSES OF THE SELECTED MOLECULES (THE
C INDICATION OF WHAT SPECIES THEY ARE HAS BEEN DEFINED HERE)
DO 930 N=1,3
IF(L.EQ.1)VN1=P1(N,MAD1)
IF(L.EQ.2)VN1=P2(N,MAD1)
IF(L.EQ.3)VN1=P3(N,MAD1)
C
IF(M.EQ.1)VN2=P1(N,MAD2)
IF(M.EQ.2)VN2=P2(N,MAD2)
IF(M.EQ.3)VN2=P3(N,MAD2)
C
930 VRC(N)=VN1-VN2
C VRC(3) CONTAIN THE THREE RELATIVE VELOCITY COMPONENTS
VR=SQRT(VRC(1)*VRC(1)+VRC(2)*VRC(2)+VRC(3)*VRC(3))
C VR IS THE RELATIVE SPEED IN A SPECIFIC COLLISION
IF(C(KV,I,J).LT.VR)C(KV,I,J)=VR
C LAST STATEMENT RESETS THE MAXIMUM RELATIVE VELOCITY FOR FURTHER
C CALCULATIONS
C
IF(KREJ.GT.100)GO TO 911

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SIM09370
SIM09380
SIM09390
SIM09400
SIM09410
SIM09420
SIM09430
SIM09440
SIM09450
SIM09460
SIM09470
SIM09480
SIM09490
SIM09500
SIM09510
SIM09520
SIM09530
SIM09540
SIM09550
SIM09560
SIM09570
SIM09580
SIM09590
SIM09600
SIM09610
SIM09620
SIM09630
SIM09640
SIM09650
SIM09660
SIM09670
SIM09680
SIM09690
SIM09700
SIM09710
SIM09720
SIM09730
SIM09740
SIM09750
SIM09760
SIM09770
SIM09780
SIM09790
SIM09800
SIM09810
SIM09820
SIM09830
SIM09840
SIM09850
SIM09860
SIM09870
SIM09880
SIM09890
SIM09900
SIM09910
SIM09920
SIM09930
SIM09940
SIM09950
SIM09960
SIM09970
SIM09980
SIM09990
SIM10000
SIM10010
SIM10020
SIM10030
SIM10040
SIM10050
SIM10060
SIM10070
SIM10080

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C	CALL RANDU(P)	SIM10090
	AVR=VR/C(KV,I,J)	SIM10100
	KREJ=KREJ+1	SIM10110
	IF(AVR.LT.P)GO TO 912	SIM10120
C	LAST STATEMENT REJECTS THE CALCULATED COLLISION	SIM10130
C		SIM10140
C	NOW A SPECIES L-M COLLISION HAS BEEN SELECTED	SIM10150
C		SIM10160
C	CALCULATE NOW THE PROBABILITY THAT SUCH A COLLISION WILL BE COUNTED	SIM10170
C	FOR THE L AND M SPECIES RESPECTIVELY	SIM10180
	LP=1	SIM10190
	LM=1	SIM10200
	CALL RANDU(P)	SIM10210
	ANM=FLOAT(NM(L))/FLOAT(NM(M))	SIM10220
	IF(ANM.GT.1.)GO TO 950	SIM10230
	IF(ANM.LT.P)MP=0	SIM10240
	GO TO 955	SIM10250
C		SIM10260
C		SIM10270
C	950 ANM=1./ANM	SIM10280
	IF(ANM.LT.P)LP=0	SIM10290
C		SIM10300
C		SIM10310
C	955 CXS=PI*(SPEC(L,2)+SPEC(M,2))*2/4.	SIM10320
	ALP=LP	SIM10330
	ALM=LM	SIM10340
C		SIM10350
	VOLUME=REG(4,KR,KS)*VOL(I)	SIM10360
CCHECK	SIM10370
	DNL=FLOAT(NM(L))/VOLUME	SIM10380
	DNM=FLOAT(NM(M))/VOLUME	SIM10390
C	USE EQ.10.3	SIM10400
	TOC(L,M)=ALP/(CXS*DNM*VR*NM(L))+ALM/(CXS*DNL*VR*NM(M))	SIM10410
C		SIM10420
C	SET THIS VALUE INTO C(KT,I,J)	SIM10430
	C(KT,I,J)=C(KT,I,J)+TOC(L,M)	SIM10440
C	SIM10450
C	SAMPLE THIS COLLISION	SIM10460
	NCOL(I,J)=NCOL(I,J)+1	SIM10470
C		SIM10480
C	FIND RELATIVE MASSES	SIM10490
	CALL RANDU(P)	SIM10500
	BB=1.-2.*P	SIM10510
	AA=SQRT(1.-BB*BB)	SIM10520
	VRC(1)=BB*VR	SIM10530
	CALL RANDU(P)	SIM10540
	BB=2.*PI*P	SIM10550
	VRC(2)=AA*COS(BB)*VR	SIM10560
	VRC(3)=AA*SIN(BB)*VR	SIM10570
C		SIM10580
C	FIND RELATIVE MASSES	SIM10590
	SM=SPEC(L,1)+SPEC(M,1)	SIM10600
	RML=SPEC(L,1)/SM	SIM10610
	RMM=SPEC(M,1)/SM	SIM10620
C		SIM10630
C	*****	SIM10640
C	CALCULATE HERE THE ACTUAL ADDRESSES OF COLLIDING MOLECULES AND SET	SIM10650
C	THEIR NEW VELOCITIES (NEW VELOCITY COMPONENTS ARE ADDED TO THE	SIM10660
C	VELOCITY OF THE CENTER OF MASS VCCM)	SIM10670
	DO 960 N=1,3	SIM10680
	IF(L.EQ.1)V1=P1(N,MAD1)	SIM10690
	IF(L.EQ.2)V1=P2(N,MAD1)	SIM10700
C	IF(L.EQ.3)V1=P3(N,MAD1)	SIM10710
	IF(M.EQ.1)V2=P1(N,MAD2)	SIM10720
	IF(M.EQ.2)V2=P2(N,MAD2)	SIM10730
C	IF(M.EQ.3)V2=P3(N,MAD2)	SIM10740
C		SIM10750
C		SIM10760
	VCCM=RML*V1+RMM*V2	SIM10770
	VCCM1=VCCM+VRC(N)*RMM	SIM10780
C	VCCM2=VCCM-VRC(N)*RML	SIM10790
		SIM10800

C	CHANGE IN VELOCITY IS INPUTED ONLY IF PROBABILITY OF COLLISION.GT.1	SIM10810
	IF(LP.NE.1)GO TO 961	SIM10820
	IF(L.EQ.1)P1(N,MAD1)=VCCM1	SIM10830
	IF(L.EQ.2)P2(N,MAD1)=VCCM1	SIM10840
C	IF(L.EQ.3)P3(N,MAD1)=VCCM1	SIM10850
C		SIM10860
	961 IF(LM.NE.1)GO TO 960	SIM10870
	IF(M.EQ.1)P1(N,MAD2)=VCCM2	SIM10880
	IF(M.EQ.2)P2(N,MAD2)=VCCM2	SIM10890
C	IF(M.EQ.3)P3(N,MAD2)=VCCM2	SIM10900
C		SIM10910
	960 CONTINUE	SIM10920
	GO TO 920	SIM10930
	900 CONTINUE	SIM10940
	WRITE(6,4545)TOC(1,1),TOC(1,2),TOC(2,1),TOC(2,2),TIME	SIM10950
	4545 FORMAT(' TIME',5E10.3)	SIM10960
C		SIM10970
	*****END OF COLLISIONS*****	SIM10980
C	NOW NEW TEMPERATURES MAY BE CALCULATED IN EACH CELL	SIM10990
C	AVERAGE VELOCITY IN CELLS	SIM11000
C		SIM11010
	WRITE(6,4547)	SIM11020
	4547 FORMAT('0 I J N1E N2E TEMPR1 TEMPR2 VAVX1	SIM11030
	1 VAVY1 VAVX2 VAVY2 NCOL',/)	SIM11040
C		SIM11050
	DO 1110 I=1,NRD	SIM11060
	DO 1110 J=1,NAD	SIM11070
	N1E=IC(1,I,J)	SIM11080
	N2E=IC(2,I,J)	SIM11090
	KAD1=IC(4,I,J)	SIM11100
	KAD2=IC(4,I,J)+N1E	SIM11110
	IF(N1E.LT.1)GO TO 1112	SIM11120
C		SIM11130
	VX1=0.	SIM11140
	VX2=0.	SIM11150
	VY1=0.	SIM11160
	VY2=0.	SIM11170
C		SIM11180
	DO 1111 IM=1,N1E	SIM11190
	MAD1=KAD1+IM	SIM11200
	IAD=IP(MAD1)	SIM11210
	VX1=VX1+P1(1,IAD)	SIM11220
	1111 VY1=VY1+P1(2,IAD)	SIM11230
	1112 IF(N2E.LE.0)GO TO 1110	SIM11240
C		SIM11250
	DO 1115 IM=1,N2E	SIM11260
	MAD2=MAD1+IM	SIM11270
	IAD=IP(MAD2)	SIM11280
	VX2=VX2+P2(1,IAD)	SIM11290
	1115 VY2=VY2+P2(2,IAD)	SIM11300
C		SIM11310
C	THE AVERAGE VELOCITIES IN THE CELL WILL RESULT-	SIM11320
	VAVX1=VX1/N1E	SIM11330
	VAVY1=VY1/N1E	SIM11340
	VAVX2=VX2/N2E	SIM11350
	VAVY2=VY2/N2E	SIM11360
	IF(I.NE.1)GO TO 1116	SIM11370
C		SIM11380
	FSN1(2,J,KR)=VAVX1+FSN1(2,J,KR)	SIM11390
	FSN1(3,J,KR)=VAVY1+FSN1(3,J,KR)	SIM11400
	FSH2(2,J,KR)=VAVX2+FSN2(2,J,KR)	SIM11410
	FSH2(3,J,KR)=VAVY2+FSN2(3,J,KR)	SIM11420
C		SIM11430
	1116 IF(I.NE.NRD)GO TO 1117	SIM11440
	FNN1(2,J,KR)=VAVX1+FNN1(2,J,KR)	SIM11450
	FNN1(3,J,KR)=VAVY1+FNN1(3,J,KR)	SIM11460
	FNN2(2,J,KR)=VAVX2+FNN2(2,J,KR)	SIM11470
	FNN2(3,J,KR)=VAVY2+FNN2(3,J,KR)	SIM11480
C		SIM11490
	1117 IF(J.NE.1)GO TO 1118	SIM11500
	FEN1(2,I)=VAVX1+FEN1(2,I)	SIM11510
	FEN1(3,I)=VAVY1+FEN1(3,I)	SIM11520

FEN2(2,I)=VAVX2+FEN2(2,I)	SIM11530
FEN2(3,I)=VAVY2+FEN2(3,I)	SIM11540
C	SIM11550
1118 IF(J.NE.NAD)GO TO 1119	SIM11560
FWN1(2,I)=VAVX1+FWN1(2,I)	SIM11570
FWN1(3,I)=VAVY1+FWN1(3,I)	SIM11580
FWN2(2,I)=VAVX2+FWN2(2,I)	SIM11590
FWN2(3,I)=VAVY2+FWN2(3,I)	SIM11600
1119 CONTINUE	SIM11610
C	SIM11620
C THERMAL VELOCITIES AND TEMPERATURES	SIM11630
ENRG1=0.	SIM11640
ENRG2=0.	SIM11650
IF(N1E.LT.1)GO TO 1131	SIM11660
DO 1130 IM=1,N1E	SIM11670
MAD1=KAD1+IM	SIM11680
IAD=IP(MAD1)	SIM11690
CX1=P1(1,IAD)-VAVX1	SIM11700
CY1=P1(2,IAD)-VAVY1	SIM11710
CZ1=P1(3,IAD)	SIM11720
1130 ENRG1=ENRG1+CX1*CX1+CY1*CY1+CZ1*CZ1	SIM11730
1131 IF(N2E.LT.1)GO TO 1150	SIM11740
DO 1140 IM=1,N2E	SIM11750
MAD2=KAD2+IM	SIM11760
IAD=IP(MAD2)	SIM11770
CX2=P2(1,IAD)-VAVX2	SIM11780
CY2=P2(2,IAD)-VAVY2	SIM11790
CZ2=P2(3,IAD)	SIM11800
C	SIM11810
C	SIM11820
1140 ENRG2=ENRG2+CX2*CX2+CY2*CY2+CZ2*CZ2	SIM11830
C	SIM11840
1150 TEMPR1=(ENRG1/N1E)*SPEC(1,1)/(3.*BOLTZ)	SIM11850
TEMPR2=(ENRG2/N2E)*SPEC(2,1)/(3.*BOLTZ)	SIM11860
C	SIM11870
IF(I.NE.1)GO TO 1151	SIM11880
FSN1(4,J,KR)=TEMPR1+FSN1(4,J,KR)	SIM11890
FSN2(4,J,KR)=TEMPR2+FSN2(4,J,KR)	SIM11900
C	SIM11910
1151 IF(I.NE.NRD)GO TO 1152	SIM11920
FNN1(4,J,KR)=TEMPR1+FNN1(4,J,KR)	SIM11930
FNN2(4,J,KR)=TEMPR2+FNN2(4,J,KR)	SIM11940
C	SIM11950
1152 IF(J.NE.1)GO TO 1153	SIM11960
FWN1(4,I)=TEMPR1+FWN1(4,I)	SIM11970
FWN2(4,I)=TEMPR2+FWN2(4,I)	SIM11980
C	SIM11990
1153 IF(J.NE.NAD)GO TO 1154	SIM12000
FEN1(4,I)=TEMPR1+FEN1(4,I)	SIM12010
FEN2(4,I)=TEMPR2+FEN2(4,I)	SIM12020
1154 CONTINUE	SIM12030
C	SIM12040
WRITE(6,4548)I,J,N1E,N2E,TEMPR1,TEMPR2,VAVX1,VAVY1,VAVX2,VAVY2,NCOS	SIM12050
11(I,J)	SIM12060
4548 FORMAT(' ',4I5,6F12.3,I7)	SIM12070
C	SIM12080
1110 CONTINUE	SIM12090
C	SIM12100
6000 CONTINUE	SIM12110
C CALCULATE AVERAGED PARAMETERS, WEIGHTED BY DFI	SIM12120
DO 6010 I=1,NRD	SIM12130
DO 6010 KPAR=1,4	SIM12140
FOH1(KPAR,I,KR,KS)=FWN1(KPAR,I)/(NIS)	SIM12150
FOH2(KPAR,I,KR,KS)=FWN2(KPAR,I)/(NIS)	SIM12160
FOE1(KPAR,I,KR,KS)=FEN1(KPAR,I)/(NIS)	SIM12170
6010 FOE2(KPAR,I,KR,KS)=FEN2(KPAR,I)/(NIS)	SIM12180
C	SIM12190
DO 6020 J=1,NAD	SIM12200
DO 6020 KPAR=1,4	SIM12210
FSN1(KPAR,J,KR)=FSN1(KPAR,J,KR)/NIS	SIM12220
FSN2(KPAR,J,KR)=FSN2(KPAR,J,KR)/NIS	SIM12230
FNN1(KPAR,J,KR)=FNN1(KPAR,J,KR)/NIS	SIM12240

```

6020 FNN2(KPAR,J,KR)=FNN2(KPAR,J,KR)/NIS
C TO PREPARE FLOWS FOR THE NEXT REGION OR SECTOR, DIVIDE F(N) BY LOCAL
C DFI AND MULTIPLY BY NEXT DFI WHEN STARTING NEW REGION
C CALCULATE HERE THE MEAN FREE PATH AND STORE INTO REG(,,)
C STOP PROGRAM IF FLOW BECOMES COLLISIONLESS OR NUMBER DENSITY IS EQUAL
C TO THE AMBIENT NUMBER DENSITY. STORE FOE1,FOE2 IN A SEPARATE FILE TO
C BE USED IN A DIFFERENT PROGRAM.
C PRINT AVERAGED RESULTS
  WRITE(6,6029)
6029 FORMAT(' ',//)
  WRITE(6,6030)NIS,KR
6030 FORMAT(' AVERAGED OUTPUT FLOWS AFTER',I5,' TIME INCREMENTS IN REGI
10N',I5)
  WRITE(6,6031)
6031 FORMAT('0      I      FEN1(1,I)      FEN2(1,I)      FWN1(1,I)      FWN2(1,I)'
1)
  DO 6033 I=1,NRD
  WRITE(6,6032)I,FEN1(1,I),FEN2(1,I),FWN1(1,I),FWN2(1,I)
6032 FORMAT(' ',I5,4F13.3)
6033 CONTINUE
  WRITE(6,6034)
6034 FORMAT('0      J      FNN1(1,J,KR)      FNN2(1,J,KR)      FSN1(1,J,KR)      FSN
12(1,J,KR)')
  DO 6036 J=1,NAD
  WRITE(6,6037)J,FNN1(1,J,KR),FNN2(1,J,KR),FSN1(1,J,KR),FSN2(1,J,KR)
6037 FORMAT(' ',I5,4F15.5)
6036 CONTINUE
C *****
C START A NEW REGION
  IF(KR.EQ.10) GO TO 7000
  KR=KR+1
  GO TO 2000
C *****
7000 CONTINUE
C *****
C FIND IF FLOW BECAME COLLISIONLESS IN THE WHOLE SECTOR
C IF POSITIVE, STORE FOE1,FOE2 IN A SEPARATE FILE AND STOP PROGRAM
C PREPARE DATA FOR THE NEXT SECTOR
  KR=1
  STOP PROGRAM IF KS WAS BOUNDED BY THE WALL
  KS=KS+1
  GO TO 1000
C *****
C IF THERE IS BACK FLOW (FWN1,FWN2) NONZERO CALCULATE NEXT ITERATION
  ITER=ITER+1
  KS=KR=1
  GO TO 3000
C *****
  WRITE(6,6099)
6099 FORMAT('1 DATA FOR TEN MOLECULES SPEC.2')
  DO 3003 I=1,10
  WRITE(6,3002) P2(1,I),P2(2,I),P2(3,I),P2(4,I),P2(5,I)
3002 FORMAT(' ',4F10.3,E18.10)
3003 CONTINUE
  GO TO 3009
3004 WRITE(6,3005)

```

```

SIM12250
SIM12260
SIM12270
SIM12280
SIM12290
SIM12300
SIM12310
SIM12320
SIM12330
SIM12340
SIM12350
SIM12360
SIM12370
SIM12380
SIM12390
SIM12400
SIM12410
SIM12420
SIM12430
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SIM12460
SIM12470
SIM12480
SIM12490
SIM12500
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SIM12570
SIM12580
SIM12590
SIM12600
SIM12610
SIM12620
SIM12630
SIM12640
SIM12650
SIM12660
SIM12670
SIM12680
SIM12690
SIM12700
SIM12710
SIM12720
SIM12730
SIM12740
SIM12750
SIM12760
SIM12770
SIM12780
SIM12790
SIM12800
SIM12810
SIM12820
SIM12830
SIM12840
SIM12850
SIM12860
SIM12870
SIM12880
SIM12890
SIM12900
SIM12910
SIM12920
SIM12930
SIM12940
SIM12950
SIM12960

```

3005 FORMAT(' NO PLACE FOR ADDITIONAL MOLECULES')
3009 CONTINUE
STOP
END

C
C

SUBROUTINE RANDU(P)
COMMON IX
IY = IX*65539
IF (IY) 5,6,6
5 IY = IY+2147483647+1
6 P = IY
P = P*.4656613E-9
IX = IY
RETURN
END

SIM12970
SIM12980
SIM12990
SIM13000
SIM13010
SIM13020
SIM13030
SIM13040
SIM13050
SIM13060
SIM13070
SIM13080
SIM13090
SIM13100
SIM13110
SIM13120

B.5 Program SIMUL - User's Guide

Preparation: Run AXSYM program. From its output data evaluate:

ALFA - The averaged angle for the continuum breakdown

($P \sim 0.05$)

TETA - Flow direction along the breakdown limit.

Flow parameters along this line - Pressure, temperature, velocity, mean free path.

Input Data:

Radius of nozzle ring	RI
Radial size of a cell	DR
Maximum radius in simulation	RP
Angle of breakdown limit	ALFA
Flow direction along (ALFA)	TETA
Averaged flow velocity along (ALFA)	Vo
Molecular weight of each species	Spec(I,1)
Molecular diameter of each species	Spec (I,2)
Mean free path along (ALFA)	FPM
Averaged Temperature (ALFA)	TEMP
Time increment	DTH
Number of time increments	NIS

Options

a. Geometry

The program is designed to run for axisymmetric ring flow.

For a two dimensional planar flow the molecular motion, collisions and flow calculation remain unchanged. The flow cross section remain

unchanged. Instead of the angle DFI the two dimensional flow requires the definition of the width of each region (or cell). To keep the number of molecules within reasonable computational limits this size has to decrease in the same manner as DFI.

The part of the program which has to be changed for this purpose is lines 230 to 250.

b. Wall flux calculations:

The program may run for the whole molecular region resulting the flux towards the wall (this part needs additional debugging). However in order to make it more efficient we may stop the program at a sector where the flow becomes collisionless. The remaining part of the flow may be regarded either as collisionless or if we define a much larger size of cells we may calculate the molecular collisions on this basis.

This part need additional analysis and programming.

Execution Commands

Without additional changes the program runs under WATFIV compiler using the following command:

```
WATFI AXSYM * (XTYPE)
```

Further developments will be required to run the program for each sector separately and the output intermediate results on the mass storage.

B.6 The Influence of the Ambient Gas

The temperature, pressure and density of the ambient gas are shown in Table 1. Because its temperature is much higher than in the jet gas, the thermal velocity of ambient gas molecules is much higher than jet molecules. the following contribution may be expected due to the ambient gas:

- a. Collisions between the "hot" ambient molecules with the "cold" jet molecules may cause an increase in the dissipation in the outer layer of the jet and increase in the flux towards the walls.
- b. For higher ambient pressures, those collisions become rare because of the low number density therefore, the influence of the collisions may decrease.

The only way to evaluate the influence of these two controversial factors is by an additional simulation program to be designed for this region. The following are the main factors to be included in this program:

Boundary Conditions:

- a. The jet side: FOE1 and FOE2 obtained from the last simulated sector (SIMUL) supply the number flux, flow velocity componetns and temperatures. These parameters are given for all points along the radius $R(I)$ at constant distances DR . In the low density domain the resolution DR is much too large compared with the expected mean free path. A different mesh has to be designed for this purpose. It is possible that one cell may be sufficient.
- b. Far Field Condition: The boundary conditions where the gas may be regarded "undisturbed" by the jet are as follows

- Jet gas molecules are allowed to go out the simulation region (these molecules will be regarded as "lost" molecules).
- Ambient gas is allowed to enter the simulated region according with their thermal velocity and number density.

c. Solid Wall Boundaries. The solid wall may be assumed to have a constant temperature T_w . Incident molecules of either species are reflected back from the wall. Different models of collisions with the wall may be employed.

- Elastic collisions 'specular reflection' (this calculation has been included in SIMUL program)
- Collisions with ideal heat transfer (diffuse reflections)
- Other models depending on the materials and surface parameters.

The collision with the wall was included as an internal routine in the program SIMUL. If the general molecular simulation contains the program proposed here the collision with the wall will be omitted from SIMUL and become the core of the additional collisionless program. Figure 25 shows the low density (collisionless) region and its boundaries.

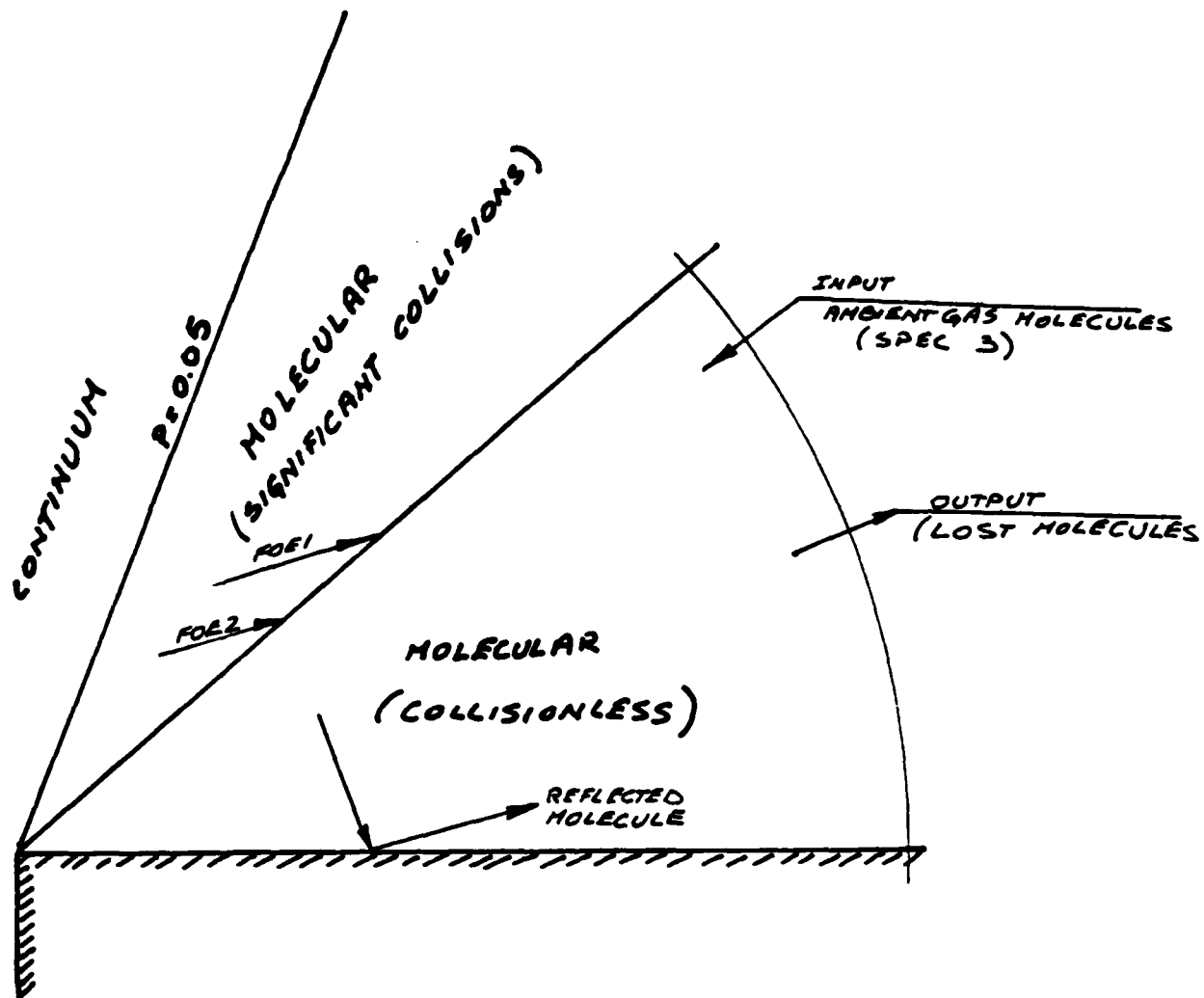


Figure 25. The Low Density Region in the Jet

SUMMARY OF REPORT

Algorithms for the continuum regime and for the region where molecular collisions are significant have been developed.

Program AXSYM contains the calculation of planar jet flow and axisymmetric ring jet flow. This program supplies data for the limits where the continuum approach become invalid and molecular approach should be employed.

Program SIMUL contains the molecular simulation for the axisymmetric ring flow. This program may run for the whole molecular region to result in the calculation of flux towards the solid wall. For a more efficient simulation it is proposed to design an additional program for the collisionless region where ambient gas may be included.

For the two dimensional flow, program SIMUL may be used after changing the definition of the cell geometry.

To run the whole program it may be required to make separate runs for each sector and store results on the mass storage.

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